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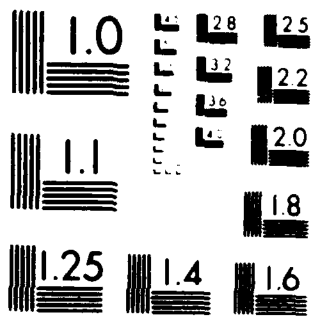

MICROCOPY RESOLUTION TEST CHART

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VOLUME II

CAD/CAM HANDBOOK FOR POLYMER COMPOSITE RELIABILITY

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U.S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 22709

D.H. Kaelble
Principal Investigator

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CAD/CAM HANDBOOK FOR POLYMER COMPOSITE RELIABILITY

VOLUME II

FIGURES AND TABLES

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Table 1-1

THE DEACON'S MASTERPIECE:

Or the Wonderful "One-Hoss-Shay."*
A Logical Story

Have you heard of the wonderful one-hoss-shay,
That was built in such a logical way
It ran a hundred years to a day,
And the, of a sudden - ah, but stay,
I'll tell you what happened without delay,

At age one hundred years to the day
There are traces of age in a one-hoss-shay
A general flavor of mild decay
But nothing local, as one may say.
There couldn't be, - for the Deacon's art
Had made it so like in very part
That there wasn't a chance for one to start.
And yet, as a whole, it is past a doubt
In another hour it will be worn out!

This morning the parson takes a drive.
All at once the horse stood still,
Close by the meet'n'-house on the hill.
-First a shiver, and then a thrill,
Then something decidedly like a spill,-
And the parson was sitting upon a rock,

-What do you think the parson found,
When he got up and stared around?
The poor old chaise in a heap or mound,
You see, of course, if you're not a dunce,
How it went to pieces at once,-
All at once, and nothing first,-
Just as bubbles do when they burst.

*Exerpts from a poem by Oliver Wendell Holmes, in "The Autocrat of the Breakfast Table," pp. 252-256, The Riverside Press, Cambridge, Mass. (1895) relating to "Structural design for reliability."

Table 1-2

Interaction Matrix Between Molecular Property and Mechanical Requirement; 3 = Strong Interaction, 2 = Medium, 1 = Negligible, - = Unknown, Σ - Sum of Interactions

Molecular Property	Mechanical Requirement T_g	E_e	τ_0	n	E_g	Σ
Volume Fraction Plasticizer	3	3	3	1	1	11
Volume Fraction Filler	2	3	2	3	1	11
Degree of Crystallinity	1	3	3	3	1	11
Molecular Weight	3	3	1	1	1	9
Crosslink Density	1	3	1	2	1	8
Chain Stiffness	3	1	0	2	1	7
Monomeric Friction Coefficient	3	1	3	0	0	7
Heterogeneity Index	2	1	2	1	1	7
Entanglement Molecular Wt	1	3	1	1	1	7
Solubility Parameter	3	1	0	0	2	6
Σ	22	22	16	14	10	

*T_g = glass temp; Modulus (E) vs time (t) = $E(t) = E_e + [E_g - E_e]\,[1 + t/\tau_0]^{-n}$ where E_e = elastomeric modulus, E_g = glass modulus, τ_0 = glass to rubber relaxation time, n = exponent.

Table 1-3
Nomenclature for Polymer Reliability Relations

Symbol	Meaning
$T_{g\infty}$	Reference glass transition defined by monomer composition.
ΣU_c	Summation of molecular molar cohesion.
Σh	Summation of molecular degrees of freedom.
$C(t)$	Time scale correction factor $C(t) = 25°C$.
T_g	Nominal T_g as affected by mechanical (tensile) stress σ, moisture concentration C_{H_2O}, and U.V. radiation effects on polymer reciprocal molecular weight (M^{-1}, number average.
a_T	Time shift factor for rheological response.
T	Test temperature.
M_i	Time dependent modulus.
M_o	Glass (solid) state modulus.
M_∞	Rubbery state modulus.
t,n	Test time and exponent.
τ_1	Relaxation time for glass to rubber transition.
τ_2	Terminal time for rubber to flow transition.
R_i	Reliability (≡ survival probability).
R_∞	Residual reliability at infinite time.
τ_o	Relaxation time for Weibull failure process.
σ_o	Stress (tensile) for Weibull failure process.
ϵ_o	Strain (tensile) for Weibull failure process.
$m(t)$, $m(\sigma)$, $m(\epsilon)$	Weibull distribution shape factors for time (t), stress (σ), and strain (ϵ) dominated failure.

Table 1-4

Weibull Strength Distributions

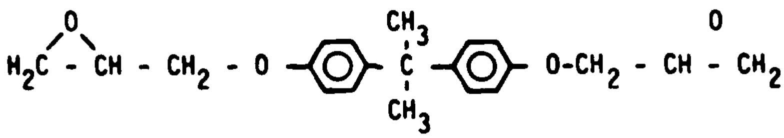
Composite Polymer		Test	Strength Distribution $R = \exp -(\sigma_b/\sigma_0)^{m(\sigma)}$	
EPON 828/CTBN % CTBN	T(°C)	Tensile	σ_0 (Kg/cm)	$m(\sigma)$
0	-150	N = 15	812	7.64
17	-150	14	679	9.78
50	-150	14	1274	15.5
0	100	15	95.6	6.82
17	100	15	42.1	8.33
50	100	15	26.6	5.44
Uniaxial Graphite/Epoxy		Interlaminar		
Herc. AS/3501-5		Shear	σ_0(Kg/cm^2)	$m(\sigma)$
23°C air + 232°C spike		N = 18	1054	7.60
100°C water + 232°C spike		16	601	2.20
Metal-Adhesive Joint Al2024T3-HT424 Epoxy SET (hr)	BET (hr)	Single Lap Shear	σ_0(Kg/cm^2)	$m(\sigma)$
0	0	N = 12	232	14.5
0	165, 449	12	184	15.4
0	808, 1023	12	165	10.0
21	0	12	208	15.0
20	669, 983	12	160	18.1
Ti-6Al-4V-HT424 Epoxy SET (hr)	BET (hr)		σ_0(Kg/cm^2)	$m(\sigma)$
0	0	N = 12	270	7.65
0	(670, 1016)	12	182	6.22
21	0	12	272	7.65
21	(591, 997)	12	202	5.35

SET = surface exposure time
BET = bond exposure time at 54°C and 195% relative humidity.

Table 1-5

Co-reactants for Three-Dimensional Epoxy-Nitrile Rubber Block Copolymers

1. Epoxy: DGEBA (Epon 828, Shell Chemical Company), 100 pbw (parts by weight), M_n = 380 gm/mole.



2. Catalyst: Piperidine - 5 pbw

3. Carboxy terminated nitrile rubber (HYCAR CTBN, B.F. Goodrich Chemical Company) - 0, 17, 29, 39, 50% by weight based on 100 pbw Epoxy + 5 pbw piperidine.

$$HOOC - \left[(CH_2 - CH = CH - CH_2)_5 - (CH_2 - \underset{\displaystyle CN}{\underset{|}{CH}}) \right]_{10} - COOH$$

M_n = 3300 - 3500 gm/mole

4. Mix items (1), (2), (3), above, degas, and cure for 16 hours at 120°C under dry N_2.

Table 1-6

Chemical Characterization of Graphite-Epoxy Prepreg Materials

		This Study		Reference System
1)	Epoxy Marix	Hercules 3501-5	Fiberite 934	NARMCO 5208
2)	Graphite Fiber	Hercules Type AS	U. Carbide T300	U. Carbide T300
3)	% Total DDS Curative by IR Spectroscopy	29.2	27.8	22.1
4)	% Free DDS Curative by Liquid Chromatography	18.1	14.5	17.8
5)	Epoxide Equivalent	205	227	173
6)	Wt% BF_3 Type Boron	0.047	0.022	0.0005
7)	Relative Degree of Cure by Liquid Chromatography	22	27	6.9
8)	Heat of Polymerization by DSC (cal/g polymer)	107	107	140

Table 1-7

Metal Joint Reliability Studies

1. Metal Adherends: Unclad 2024-T3 aluminum alloy surface treated by standard FPL sulfuric chromate etch and T8-6Al-4V titanium alloy treated by standard phosphate fluoride cleaning process. Coupon size 0.063 in. thick, 1 in. wide, and 4 in. long.

2. Adhesive: HT 424 epoxy-phenolic film adhesive (from American Cyanamid) with glass fiber carrier and standard weight 0.0135 ± 0.005 lb/sq. ft. Unfilled HT 424 primer with parts A and B used with adhesive.

3. Bonding Process: Treated metal coupons spray primed with 0.001 in. thickness HT 424 primer solution using clean dry argon carrier gas. Primer layers dried 30 min ambient 23°C and 60 min at 66°C. An adhesive film is placed in the 1.000 in. × 0.500 in. overlap between two meal adherends. Six such joints are aligned in a bonding jig with the glass carrier acting to provide constant glue line thickness 0.008 in. Cure cycles with 60 min temperature rise to 171°C and 60 min cure cycle at 171° followed by cooling to room temperature.

4. Tensile Lap Shear Testing: 1.5 in. × 1.0 in. × 0.063 in. aluminum alignment shims bonded to eliminate offset. Tests at 23°C using 0.01 in./min Instron crosshead rate and 4.5 in. jaw separation.

Table 2-1

Detailed Listing of Characterization Methods
(Sheet 1 of 4)

1. Chemical Quality Assurance
   1. HPLC (high performance liquid chromatography)
   2. GC/MS (gas chromatography/mass spectroscopy)
   3. FTIR (Fourier transform infrared spectroscopy)
   4. NMR (nuclear magnetic resonance spectroscopy)
   5. Elemental Analysis
   6. Surface Analysis

2. Processability Testing
   1. DSC (differential scanning calorimetry)
   2. TMA (thermal mechanical analysis)
   3. DMA (dynamic mechanical analysis)
   4. TGA (thermal gravimetric analysis)
   5. SEA (surface energy analysis)

3. Cure Monitoring and Management
   1. Temperature/Pressure/Vacuum
   2. AC Dielectrometry
   3. DC Conductivity
   4. Acoustic Emission

4. Non-destructive Evaluation
   1. US (ultrasonic) immersion C-scan reflector plate
   2. US immersion C-scan through transmission
   3. US contact through transmission
   4. US contact pulse-echo
   5. Fokker bond tester
   6. 210 sonic bond tester
   7. Sondicator
   8. Harmonic bond tester
   9. Neutron radiography
   10. Low KV x-ray
   11. Coin tap test
   12. Acoustic emission
   13. Thermography

5. Surface NDE
   1. Ellipsometry
   2. Surface Potential Difference (SPD)
   3. Photoelectron Emission (PEE)
   4. Surface Remission Photometry (SRP)

Table 2-1
(Sheet 2 of 4)

6. Performance and Proof Testing

The following presents a listing of the properties of plastics reported in this book, the ASTM test numbers and the equivalent DIN test:

ASTM-DIN Test Equivalents

	Units of Measure			Test	
	English	Metric	SI	ASTM	DIN
Processing					
1. Processing Methods	°F	°C			
2. Comp'n Molding Temp	°F	°C			
3. Inject Stock Melt Temp	°F	°C			
4. Extrusion Temp	°F	°C			
5. Bulk Factor				D1895	D[53466]
6. Linear Mold Shrinkage	in./in.			D955	D[53464]
7. Melt Flow		g/10 min		D1238	D[53735]
8. Melting Point	°F1	°C			
9. Density	lb/ft^3	g/cm^3	Mg/m^3	D792	D[53479]
10. Specific Volume	$in.^3/lb$	cm^3/g	m^3/Mg	D792	D[53479]
Mechanical Properties					
11. Tensile Str. yield	$10^3 lb/in.^2$	$10^2 kg/cm^2$	MPa	D638	
12. Tensile Str. Break	$10^3 lb/in.^2$	$10^2 kg/cm^2$	MPa	D638	D[53455]
13. Tensile Str. low temp	$10^2 lb/in.^2$	$10^2 kg/cm^2$	MPa	D638	D[53455]
14. Tensile Str. high temp	$10^3 lb/in.^2$	$10^2 kg/cm^2$	MPa	D638	D[53455]
15. Elongation %, yield				D638	D[53455]
16. Elongation %, break				D638	D[53455]
17. Tensile Modulus	$10^5 lb/in.^2$	$10^4 kg/cm^2$	GPa	D638	D[53457]
18. Flexural Str. yield	$10^3 lb/in.^2$	$10^2 kg/cm^2$	MPa	D790	D[53452]
19. Flexural Modulus	$10^5 lb/in.^2$	$10^4 kg/cm^2$	GPa	D790	D[53457]
20. Stiffness in Flex.	$10^5 lb/in.^2$	$10^4 kg/cm^2$	GPa	D747	
21. Compressive Str.	$10^3 lb/in.^2$	$10^2 kg/cm^2$	MPa	D695	D[53454]
22. Izod. notched R.T.	ft lb/in.	Kg cm/cm	kJ/m	D256	
23. Izod. low temp	ft lb/in.	Kg cm/cm	kJ/m	D256	
24. Hardness	(test)				

Table 2-1
ASTM-DIN Test Equivalents
(Sheet 3 of 4)

	Units of Measure			Test	
	English	Metric	SI	ASTM	DIN
Thermal Properties					
25. Thermal Conductivity	BTU in./hr ft^2 °F	10^{-4} cal/sec cm^2 °C/cm	W/Km	C177	D[52612]
26. Specific Heat	BTU in./hr ft^2	cal/g°C	kJ/kg K	C351	
27. Linear Therm. Expan	10^6 in./in.°F	10^{-5} mm/mm	K	D696	D[52328]
28. Vicat Soft Point	°F	°C		D1525	D[53460]
29. Brittle Temp	°F	°C		D746	
30. Continuous Svc Temp	°F	°C			
31. Defl Temp 264 lb/in.^{2},	18.5 kg/cm^2 °F	1.81 MPa °C		D648	D[53461]
32. Defl Temp 66 lb/in.^{2},	4.6 kg/cm^2 °F	0.45 MPa °C		D648	D[53461]
33. U.L. Temp Index		°C/mm			
Electrical Properties					
34. Volume Resistivity		Ohm cm		D257	D[53482]
35. Surface Resistivity		Ohm		D257	D[53482]
36. Insulation Resistance		Ohm		D257	D[53482]
37. Dielectric Strength	V/10^{-3} in.	kV/mm	MV/m	D149	D[53481]
38. Dielectric Constant	50-100 Hz			D150	D[53483]
39. Dielectric Constant	10^2 Hz			D150	D[53483]
40. Dielectric Constant	10^4 Hz			D150	D[53483]
41. Dissipation Factor	50-100 Hz			D150	D[53483]
42. Dissipation Factor	10^3 Hz			D150	D[53483]
43. Dissipation Factor	10^4 Hz			D150	D[53483]
Optical Properties					
44. Refractive Index, Sodium D				D542	D[53491]
45. Clarity					
Environmental Properties					
46. Water Absorp. %, 24 hr				D570	D[53473]
47. Equil. Water Content %				D570	D[53473]

Table 2-1

(Sheet 4 of 4)

7. Durability Analysis and Service Life Prediction (Some Current Programs)

   1. U.S. Army Composite Materials Research Program (AMMRC).

   2. AFML, "Processing Science of Epoxy Resin Composites, Contract No. F33615-80-C-5021.

   3. AFML/ARPA, "Quantitative NDE, Contract No. F33615-74-C-5180.

   4. AFML, "Integrated Methodology for Adhesive Bonded Joint Life Predictions," Contract No. F-33615-79-C-5088.

Table 2-2

Standard Units and Conversion Factors

ASTM TEST DESCRIPTIONS AND UNITS

Metric Units	Multiply By (To Convert)	SI Units	Multiply By (To Convert)	English Units	Property	SI Units	Multiply By (To Convert)	English Units	Multiply By (To Convert)	Metric Units
g/cm^3	1.0	Mg/m^3	0.016	lb/ft^3	Density	Mg/m^3	62.5	lb/ft^3	0.016	g/cm^3
kgf/cm^2	10.198	MN/m^2 or MPa	0.0069	lb/in^2	Tensile Strength	MN/m^2 or MPa	144.93	lb/in^2	0.0703	kgf/cm^2
kgf/cm^2	10.198	MN/m^2 or MPa	0.0069	lb/in^2	Tensile Modulus	MN/m^2 or MPa	144.93	lb/in^2	0.0703	kgf/cm^2
kgf/cm^2	10.198	MN/m^2 or MPa	0.0069	lb/in^2	Flexural Strength	MN/m^2 or MPa	144.93	lb/in^2	0.0703	kgf/cm^2
kgf/cm^2	10.198	MN/m^2 or MPa	0.0069	lb/in^2	Flexural Strength	MN/m^2 or MPa	144.93	lb/in^2	0.0703	kgf/cm^2
kgf/cm^2	10.198	MN/m^2 or MPa	0.0069	lb/in^2	Compressive Strength	MN/m^2 MPa	144.93	lb/in^2	0.0703	kgf/cm^2
kgf cm/cm	10.198	kJ/m	0.0534	ft lb/in	Izod	kJ/m	18.73	ft lb/in	5.44	kgf cm/cm
kgf cm/cm	101.936	kJ/m^2	0.021	ft lb/in^2	Charpy Impact	kJ/m^2	47.62	ft lb/in^2	2.141	kgf cm/cm^2
cal/sec cm C	23.88	W/K m	0.144	BTU in/hr ft^2 F	Thermal Conductivity	W/Km	6.944	BTU in/hr ft^2 F	3.45x10^{-4}	cal/sec cm C
cal/g C	0.239	kJ/kgK	4.187	BTU/lb F	Specific Heat	kJ/kgK	0.239	BTU/lb F	1.0	cal/g C
cm/cm C	1.0	m/m K	1.8	in/in F	Linear Expansion	m/m K	0.555	in/in F	1.8	cm/cm C
kV/mm	1.0	MV/m	0.0394	V/10^{-3} in	Dielectric Strength	MV/m	25.381	V/10^{-3} in	0.0394	kV/mm

Temperature Conversion

°F - °C - (°F 32) ÷ 1.8 °C - °F - (°C x 1.8) + 32 °C - °K - °C + 273.15

Special names and symbols for a few typical SI units are listed below:

Quantity	Name	Symbol
frequency	Hertz	Hz
power	Watt	W
electrical/resistance	Ohm	Ω
electrical/potential	Volt	V
force	Newton	N
pressure	Pascal	Pa
energy, work	Joule	J
length	meter	m
mass	kilogram	kg
time	second	s
thermodynamic/temperature	Kelvin	K

The following table lists SI units prefixes for decimal multiplication and submultiples

Factor	Prefix	Symbol
10^{18}	exa	E
10^{15}	peta	P
10^{12}	tera	T
10^{9}	giga	G
10^{6}	mega	M
10^{3}	kilo	k
10^{2}	hecto	h
10^{1}	deka	da
10^{1}	deci	d
10^{-2}	centi	c
10^{-3}	milli	m
10^{-6}	micro	μ
10^{-9}	nano	n
10^{-12}	pico	p
10^{-15}	femto	f
10^{-18}	atto	a

Table 2-3

Detailed Listing of Characterized Properties

1. Chemical Quality Assurance
   1. Chemical composition
   2. Degree of cure
   3. Molecular weight distribution
   4. Number average molecular weight
   5. Weight average molecular weight
   6. Entanglement molecular weight

2. Processability
   1. Gel point
   2. Gel faction
   3. Crosslink molecular weight
   4. Glass temperat.re
   5. Melt (flow) temperature
   6. Dynamic storage modulus
   7. Dynamic loss modulus

3. Cure Monitoring
   1. Temperature/pressure/vacuum
   2. Dynamic dielectric constant
   3. Dielectric loss factor
   4. DC conductivity

4. Nondestructive Evaluation
   1. Internal stress distributions
   2. Damage zone size
   3. Crack growth rate

5. Performance and Proof Testing
   1. Stress and environment dependent T_g
   2. Stress and environment dependent T_m
   3. Isothermal stress-strain-time-response
   4. Strength distribution
   5. Extensibility distribution
   6. Fracture energy distribution

6. Combined Bonding and Failure Testing
   1. Surface energy
   2. Surface chemistry
   3. Surface morphology
   4. Surface roughness

Table 2-4

Classification of Chromatographic Methods

I. Gas Chromatography (GC)

- Gas liquid (GLC)
- Gas solid (GSC)

II. High Performance Liquid Chromatography (HPLC)

- A. Planar Chromatography
  - Thin layer (TLC)
  - Paper (PC)
- B. Column Chromatography
  - Exclusion (EC)
    - Gel Permeation (GPC)
    - Gel filtration (GFC)
  - Liquid-solid or adsorption (LSC)
  - Liquid-liquid or partition (LLC)
  - Bonded phase (BPC)
  - Ion exchange (IEC)

From: H.M. McNair, American Laboratory, May 1980, pp. 33-44.

Table 2-5

Decision Matrix of Surface Characterization Methods for Reinforcing Fiber Coatings (35 to 70 nm thickness)

4 = Excellent
3 = Acceptable
2 = Marginal
1 = Unacceptable
0 = No Information

	Coating Durability	Molecular Orientations	Surface Concentration of Components	Surface Coatage Uniformity	Fiber Curvatures	Adhesion Strength	Thickness Uniformity	Average Coating Thickness	Row Ave.
Surface Energy Analysis	3	4	3	4	4	2	1	1	2.75
Scanning Elect. Mic. + EDAX	4	1	1	4	4	1	4	1	2.5
Electron Spect. for Chem. Anal.	4	4	4	1	1	1	1	1	2.13
ASTM Adhesion Test	4	1	1	1	1	4	1	1	1.75
Fourier Transform IR	2	2	3	1	1	1	1	1	1.50
Optical Microscopy	1	1	1	1	1	1	1	1	1.0
Secondary Ion Mass Spec.	1	1	1	1	1	1	1	1	1.0
Laser Microprobe Mass Analyser	1	1	1	1	1	1	1	1	1.0
Raman Microspectroscopy	1	1	1	1	1	1	1	1	1.0
Col Ave.	2.33	1.78	1.78	1.67	1.67	1.44	1.33	1.00	

Table 2-6

Decision Matrix Between Nondestructive Evaluation (NDE)
Built-In Defects in Laminate Panels

Direction of Decreasing Corelation:
0 = Defect Not Detected;
1 = Partial Detection;
2 = Detected

Built-In Defects in Laminate Panels	(a) Immersion C-Scan Reflector Plate	(b) 210 Sonic Bond Tester	(c) Immersion C-Scan Through Transmission	(d) Fokker Bondtester	(e) Contact Through Transmission	(f) Contact Pulse-Echo Pulse-Echo	(g) Immersion C-Scan Pulse-Echo	(h) Sonicator	(i) Harmonic Bond Tester	(j) Neutron Radiography	(k) Coin Tap Test	(l) Low KV X-ray	Row Ave.
(1) Void	2	2	2	2	2	2	2	2	2	2	1	0	1.75
(2) Void (C-14 repair)	2	2	2	2	2	2	2	2	2	2	1	0	1.75
(3) Void (9309 repair)	2	2	2	2	2	2	2	2	2	2	1	0	1.75
(4) Corroded Bond	2	2	2	2	2	2	1	1	1	2	1	2	1.67
(5) Lack of Bond (skin to adhesive)	2	2	2	2	2	2	2	2	2	0	1	0	1.58
(6) Porous Adhesive	2	2	2	0	2	2	2	0	2	2	0	2	1.50
(7) Manufacturer's Separator Sheet	2	1	2	2	1	0	2	2	0	1	0	0	1.08
(8) Burned Adhesive	2	2	2	2	2	2	1	0	0	0	0	0	1.08
(9) Thick Adhesive (1, 2, 3 ply)	2	2	1	2	0	0	0	0	0	0	0	0	0.58
Col. Ave.	2.00	1.89	1.89	1.78	1.67	1.56	1.56	1.22	1.22	1.22	0.56	0.44	

Column group heading: Nondestructive Test (NDT) Method

Table 2-7

Decision Matrix Between Nondestructive Evaluation (NDE)
Defects in Honeycomb Structures

Direction of Decreasing Correlation: 0 = Defect Not Detected; 1 = Partially Detected; 2 = Detected

Built-In Defects in Honeywell Structure	Nondestructive Test (NDT) Method: (a) Neutron Radiography	(b) Coin Tap Test	(c) Contact Through Transmission	(d) Immersion C-Scan Pulse-Echo	(e) Immersion C-Scan Through Transmission	(f) Fokker Bondtester	(g) Low KV X-Ray	(h) Harmonic Bond Tester	(i) 210 Sonic	(j) Sondicator	(k) Contact Pulse-Echo	(l) Contact Shear Wave	Row Ave.
(1) Void (Foam to Closure)	2	2	2	2	2	2	2	2	2	2	2	0	1.83
(2) Void (Adhesive to Skin)	2	2	2	2	2	2	2	2	2	2	[illegible]	0	1.67
(3) Inadequate Tie-In of Foam to Core	2	2	2	20	2	2	2	2	2	2	0	0	1.50
(4) Void (Adhesive to Core)	2	2	2	2	2	0	2	2	0	0	0	0	1.33
(5) Separator Sheet (Skin to Adhesive	2	2	2	2	2	0	0	1	0	0	1	0	0.92
(6) Water Intrusion	2	2	2	0	2	0	2	0	0	0	0	0	0.83
(7) Crushed Core (After Bonding)	1	2	1	1	1	1	2	1	0	0	0	0	0.83
(8) Inadequate Foam Depth At Closure	2	1	0	0	0	2	2	0	1	2	0	0	0.83
(9) Separator Sheet (Adhesive to Core)	2	2	0	2	1	0	0	0	0	0	2	0	0.75
(10) Chem-Mill Step Void	2	0	0	0	0	0	0	0	0	0	0	0	0.17
Col. Ave.	1.90	1.60	1.30	1.30	1.20	1.10	1.00	1.00	0.9	0.8	0.7	0	

Table 3-1

Properties of the Elements
(Sheet 1 of 2)

Code No.	Z	SY	W G/Mole	D 10^5 J/Mole	X	R 10^{-10} m	V	MV	S
1	1	H	1.008	4.35	2.20	0.32	1	1	3.13
2	3	LI	6.941	1.11	0.98	1.23	1	1	0.81
3	3	BE	9.012	(2.28)	1.57	0.90	2	2	2.22
4	5	B	10.81	(2.53)	2.04	0.82	3	3	3.66
5	6	C	12.01	3.48	2.55	0.77	4	4	5.19
6	7	N	14.01	1.61	3.04	0.75	3	5	6.67
7	8	O	16.00	1.39	3.44	0.73	2	2	2.74
8	9	F	19.00	1.53	3.98	0.72	1	1	1.39
9	11	NA	22.99	0.753	0.93	1.54	1	1	0.65
10	12	MG	24.31	(0.971)	1.31	1.36	2	2	1.47
11	13	AL	26.98	(2.06)	1.61	1.18	3	3	2.54
12	14	SI	28.09	1.77	1.90	1.11	4	4	3.60
13	15	P	30.97	2.15	2.19	1.06	5	5	4.72
14	16	S	32.06	2.13	2.58	1.02	6	6	5.88
15	17	CL	35.45	2.43	3.16	0.99	1	7	7.07
16	19	K	39.09	0.552	0.82	2.03	1	1	0.49
17	20	CA	40.08	(1.15)	1.00	1.74	2	2	1.15
18	21	SC	44.96	(2.58)	1.36	1.44	3	3	2.08
19	22	TI	47.90	(2.64)	1.54	1.32	4	4	3.03
20	23	V	50.94	(3.36)	1.63	1.22	5	5	4.10
21	24	CR	52.00	(2.38)	1.66	1.18	3	6	5.08
22	25	MN	54.94	(1.43)	1.55	1.17	2	7	5.98
23	26	FE	55.85	(2.03)	1.83	1.17	3	3	2.56
24	27	CO	58.93	(2.20)	1.88	1.16	2	3	2.59
25	28	NI	58.70	(2.12)	1.91	1.15	2	3	2.61
26	29	CU	63.55	(1.72)	1.90	1.17	2	2	1.71
27	30	ZN	65.38	(0.653)	1.65	1.25	2	2	1.60
28	31	GA	69.72	(1.36)	1.81	1.26	3	3	2.38
29	32	GE	72.59	1.57	2.01	1.22	4	4	3.28
30	33	AS	74.92	1.34	2.18	1.20	3	5	4.17
31	34	SE	78.96	1.84	2.55	1.16	4	6	5.17
32	35	BR	79.90	1.93	2.96	1.14	1	7	6.14
33	37	RB	85.47	0.519	0.82	2.16	1	1	0.46
34	38	SR	87.62	(1.05)	0.95	1.91	2	2	1.05
35	39	Y	88.91	(2.74)	1.22	1.62	3	3	1.85
36	40	ZR	91.22	(3.45)	1.33	1.45	4	4	2.76
37	41	NB	92.91	(4.85)	1.60	1.34	5	5	3.73

Table 3-1

Properties of the Elements
(Sheet 2 of 2)

Code No.	Z	SY	W G/Mole	D 10^5 J/Mole	X	R 10^{-10} m	V	MV	S
38	42	MO	95.94	(4.30)	2.16	1.30	6	6	4.62
39	43	TC	98.0	(3.35)	1.90	1.27	7	7	5.51
40	44	RU	101.07	(3.35)	2.20	1.25	3	8	6.40
41	45	RH	102.91	(3.24)	2.28	1.25	3	4	3.20
42	46	PD	106.4	(1.93)	2.20	1.28	2	4	3.13
43	47	AG	107.87	(1.44)	1.93	1.34	1	1	0.75
44	48	CD	112.41	(0.552)	1.69	1.48	2	2	1.35
45	49	IN	114.82	(1.18)	1.78	1.44	3	3	2.08
46	50	SN	118.69	1.43	1.96	1.41	4	4	2.84
47	51	SB	121.75	1.26	2.05	1.40	3	5	3.57
48	52	TE	127.60	1.38	2.10	1.36	4	6	4.41
49	53	I	126.90	1.51	2.66	1.33	1	7	5.26
50	55	CS	132.91	0.448	0.79	2.35	1	1	0.43
51	56	BA	137.33	(1.12)	0.89	1.98	2	2	1.01
52	57	LA	138.91	(2.48)	1.10	1.69	3	3	1.78
53	72	HF	178.49	(4.72)	1.30	1.44	4	4	2.78
54	73	TA	180.95	(5.56)	1.50	1.34	5	5	3.73
55	74	W	183.85	(5.61)	2.36	1.30	6	6	4.62
56	75	RE	186.21	(3.97)	1.90	1.28	7	7	5.47
57	76	OS	190.2	(3.64)	2.20	1.26	4	8	6.35
58	77	IR	192.22	(3.48)	2.20	1.27	4	6	4.72
59	78	PT	195.09	(2.79)	2.28	1.30	4	4	3.08
60	79	AU	196.97	(1.86)	2.54	1.34	3	3	2.24
61	80	HG	200.59	(0.301)	2.00	1.49	2	2	1.34
62	81	TL	204.37	(0.866)	2.04	1.48	1	3	2.03
63	82	PB	207.2	(0.992)	2.33	1.47	2	4	2.72
64	83	BI	209.0	(1.03)	2.02	1.46	3	5	3.42
65	90	TH	232.04	(3.42)	1.30	1.65	4	4	2.42
66	92	U	238.03	(3.56)	1.38	1.42	6	6	4.22
67	94	PU	244.0	(2.29)	1.28	1.21	4	6	4.96
68	7	(N2)/2	14.01	4.73	3.04	0.55	3	5	6.67
69	8	(O2)/2	16.00	2.01	3.44	0.62	2	2	2.74

Table 3-2

Comparison of Single Bond Energies

Element	Group	Single Bond Energy (kcal/mol) Ref. 2	Eq. (2) (C.N.=12)	Ratio
Lithium	IA	25.6	6.3	4.06
Sodium	IA	18	4.3	4.19
Potassium	IA	13.2	3.3	4.00
Rubidium	IA	12.4	3.4	3.65
Cesium	IA	10.7	3.0	3.57
				3.89 ± 0.27
Boron	IIIB	25.0	15.1	1.66
Germanium	IVB	37.6	13.2	2.85
Arsenic	VB	32.1	9.5	3.38
Tin	IVB	34.2	11.4	3.00
Antimony	VB	30.2	10.6	2.85
				2.75 ± 0.65

Table 3-3

Lattice Types and Packing Factors

Lattice Type	Coordination Number	Packing Factor (C)
Face centered cubic	12	1.414
Body centered cubic	8	1.299
Simple cubic	6	1.000
Tetrahedral	4	0.650

Table 3-4

Calculation of Heat of Formation for BeO, TiO_2, and Al_2O_3

```
Z, SY, W, D/1E5, X, R/1E-10, V, PH =
 4 BE 9.012  2.28  1.57  0.9  2  7
 8  0  16  1.39  3.44  0.73  2  2
 To continue press ENTER
 ?
 Chemical Analysis:
 Bonding          Bond         % Ionic      Bond         Moles
Elements         Energy        Energy      Length
A     B          (J/mole)                  (M*1E-10)
BE    BE         228000        0            1.8           -1
(02)/2(02)/2     201000        0            1.24          -1
BE    0          520951        64.776       1.4617         2
Total            612902                                    0
To continue press ENTER
Z, SY, W, D/1E5, X, R/1E-10, V, PH =
 22 TI 47.0  2.64  1.54  1.32  4  7
 8  0  16  1.39  3.44  0.73  2  2
 To continue press ENTER
 ?
 Chemical Analysis:
 Bonding          Bond         % Ionic      Bond         Moles
Elements         Energy        Energy      Length
A     B          (J/mole)                  (M*1E-10)
TI    TI         264000        0            2.64          -2
(02)/2(02)/2     201000        0            1.24          -2
TI    0          549865        63.3547      1.879          4
Total            1.26946E+06                               0
To continue press ENTER
Z, SY, W, D/1E5, X, R/1E-10, V, PH =
 13 AL 26.98  2.06  1.61  1.18  3  7
 8  0  16  1.39  3.44  0.73  2  2
 To continue press ENTER
 ?
 Chemical Analysis:
 Bonding          Bond         % Ionic      Bond         Moles
Elements         Energy        Energy      Length
A     B          (J/mole)                  (M*1E-10)
AL    AL         206000        0            2.36          -3
(02)/2(02)/2     201000        0            1.24          -3
AL    0          495669        65.1986      1.7453         6
Total            1.75301E+06                               0
To continue press ENTER
? -
```

Table 3-5

Comparison of Calculated and Experimental Heats of Formation for Oxides

Compound	$-\Delta H_f$(calc.) (10^5 J/mole)	$-\Delta H_f$ (Ref. 7) (10^5 J/mole)	Difference (10^5 J/mole)
Al_2O_3	17.5	16.3	1.20
Fe_2O_3	13.1	11.2	1.90
TiO_2	12.7	9.11	3.59
MgO	8.13	5.20	2.93
SiO_2	7.91	8.56	-0.65
BeO	6.13	6.10	0.03
MoO_2	5.08	5.43	-0.35
WO_2	3.26	5.70	-2.44
Au_2O_3	2.83	-0.80	3.63
SeO_2	1.82	2.29	-0.47
		Sum:	0.94
		Std. Dev:	± 2.04

Table 3-6

Comparison of Calculated and Experimental Heats of Formation for Chlorides

Compound	$-\Delta H_f$(calc.)	$-\Delta H_f$ (Ref. 7) (10^5 J/mole)	Difference
$AlCl_3$	6.95	6.95	0.0
$FeCl_3$	5.12	4.05	1.07
$TiCl_4$	10.1	7.50	2.60
MgCl	3.30	6.41	-3.11
$SiCl_4$	6.12	6.10	0.02
$BeCl_2$	4.87	5.11	-0.24
$MoCl_4$	3.86	3.30	0.56
$AuCl_3$	1.11	1.18	-0.07
		Sum:	0.10
		Std. Dev:	± 1.60

Table 3-7

Calculation of the Oxidation Dilation Factor ϕ for Metals

Oxide	Calculated (for Z = 12)			Exper. (7,8)	
	V(Me) (CC)	$V(MeO_x)$ (CC)	ϕ	$V(MeO_x)$ (CC)	ϕ
K_2O	57.02	20.55	0.36	40.6	0.45
BaO	26.45	13.00	0.49	26.8	0.67
MgO	8.57	6.34	0.74	11.3	0.81
Al_2O_3	11.19	11.32	1.01	25.7	1.28
TiO_2	7.84	8.48	1.08	18.7	1.78
Fe_2O_3	10.92	11.52	1.05	30.5	2.14
Ta_2O_5	16.40	20.31	1.24	53.9	2.50
Nb_2O_5	16.40	20.60	1.26	59.5	2.68
MoO_3	7.49	11.96	1.60	30.7	3.30
WO_3	7.49	12.30	1.64	32.4	3.35

$$\phi = \frac{\text{molecular volume of metal compound } MeX_x}{\text{atomic volume of equal moles of metal Me}}$$

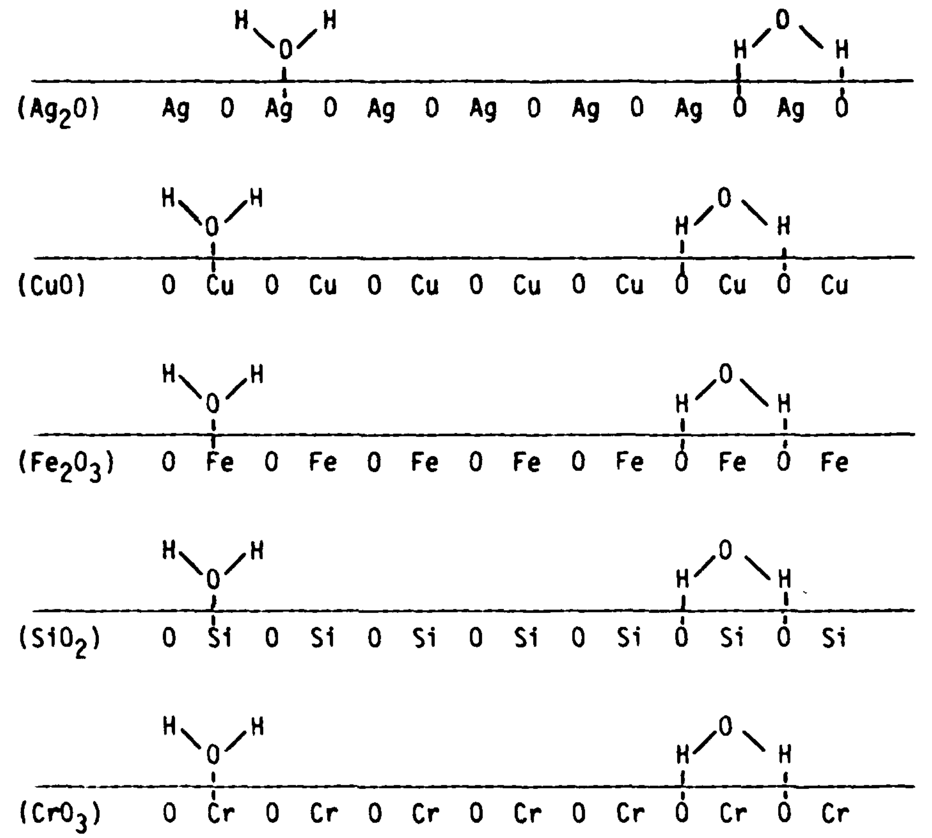
Table 3-8

Correlation Between Metal Oxidation State and IEPS

Oxide	IEPS Range (pH Units)	Acid-Base Character
M_2O	$pH > 11.5$	strong base
MO	$8.5 < pH < 12.5$	intermediate base
M_2O_3	$6.5 < pH < 10.4$	weak base
MO_2	$0 < pH < 7.5$	intermediate acid
M_2O_5, MO_3	$pH < 0.5$	strong acid

Table 3-9

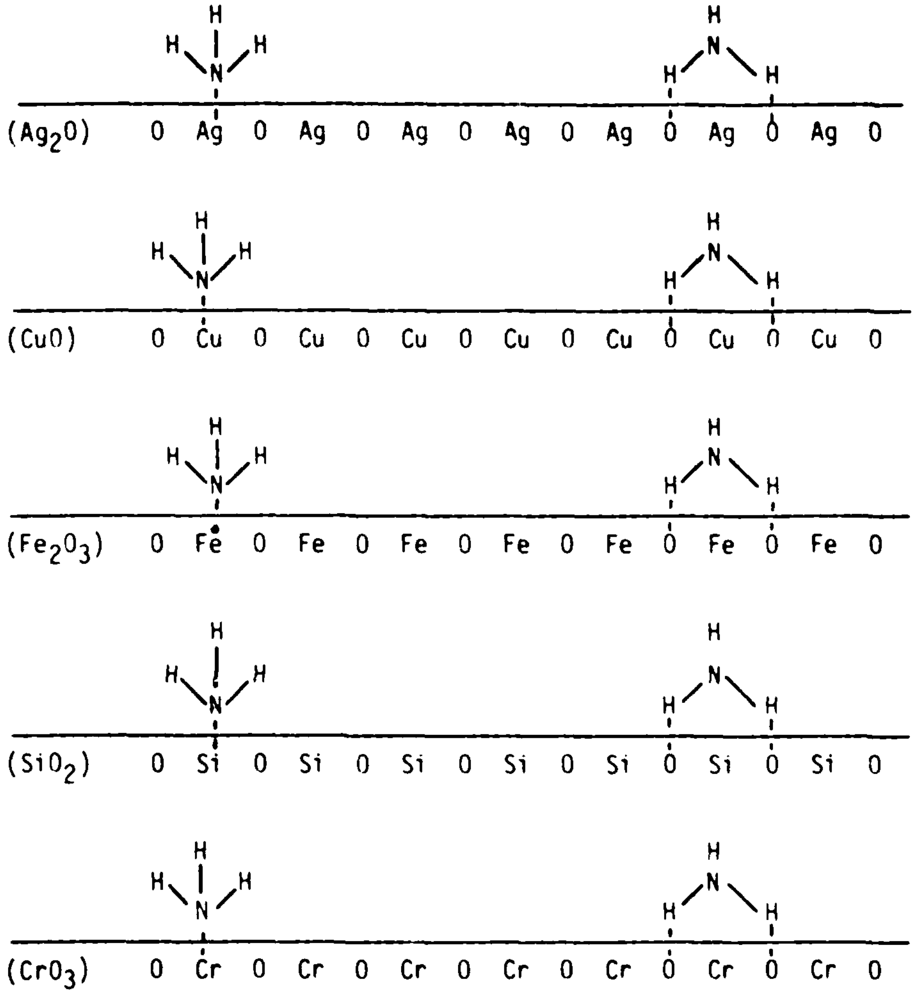
Coulomb Bond Energies Between Water and Various Oxides



Adsorbate: H_2O	Monobacic		Diacid	
Substrate Oxide	U_M(kJ/mole)	U_N	U_M	U_N
Ag_2O	11.8	2.4	46.5	9.6
CuO	25.7	5.2	46.5	9.5
Fe_2O_3	38.5	7.1	46.5	9.3
SiO_2	53.0	10.6	46.5	9.3
CrO_3	76.6	16.2	46.5	9.2

Table 3-10

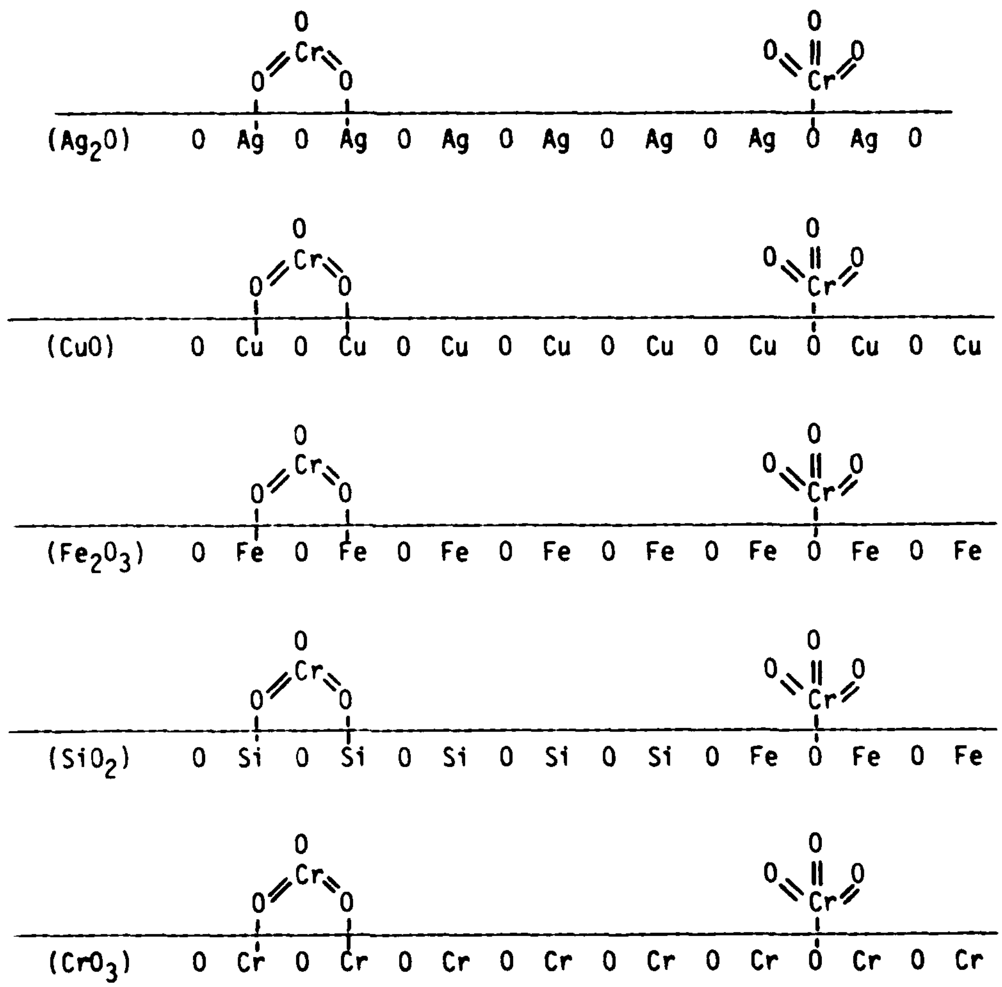
Coulomb Bond Energies Between Ammonia and Various Oxides



Adsorbate: NH_3	Monobacic		Diacid	
Substrate Oxide	U_M(kJ/mole)	U_N	U_M	U_N
Ag_2O	17.5	2.0	46.5	9.6
CuO	38.1	4.3	46.5	9.5
Fe_2O_3	57.2	6.4	46.5	9.3
SiO_2	78.7	8.8	46.5	9.3
CrO_3	113.8	13.4	46.5	9.2

Table 3-11

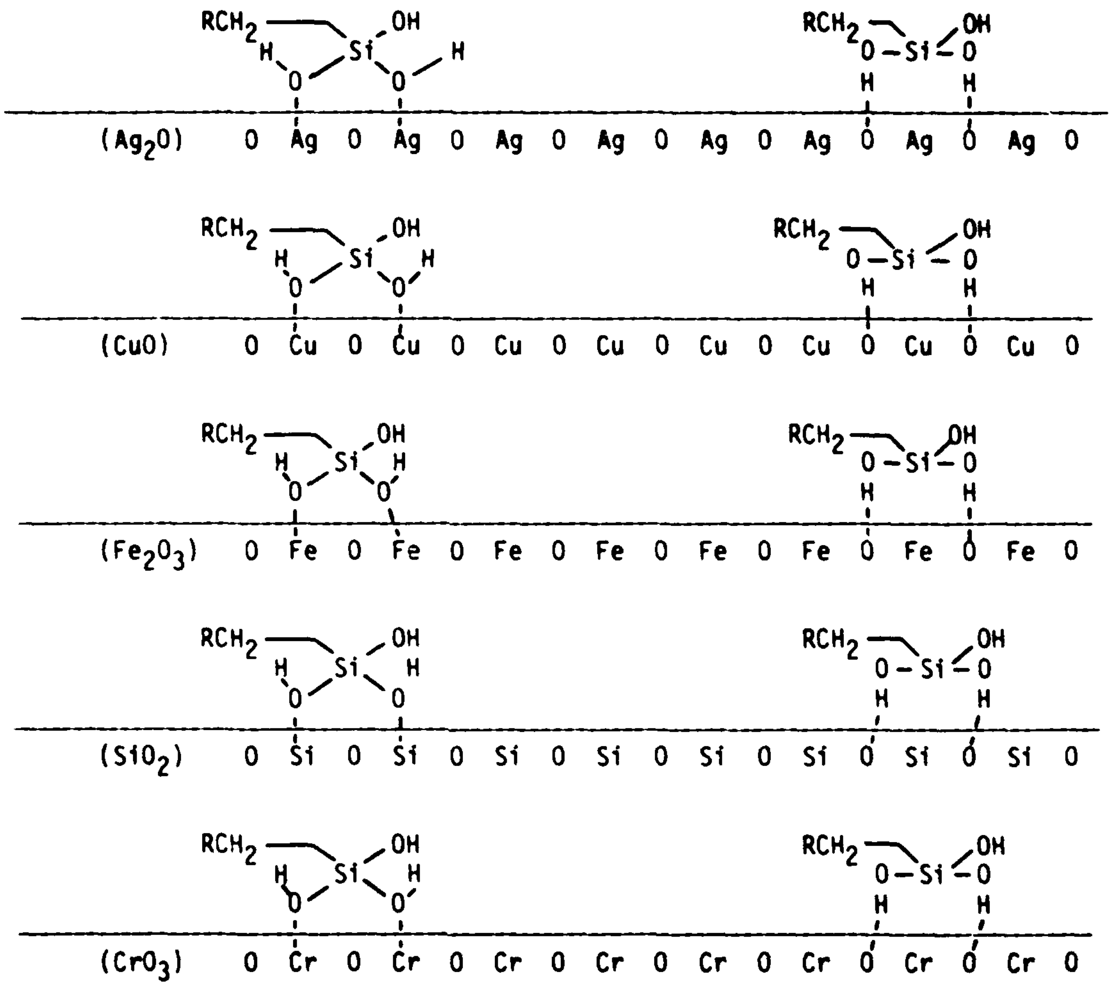
Coulomb Bond Energies Between Chromium Trioxide and Various Oxides



Adsorbate: CrO_3	Dibasic		Monoacid	
Substrate Oxide	U_M(kJ/mole)	U_N	U_M	U_N
Ag_2O	24.9	8.8	76.6	27.1
CuO	40.9	14.2	76.6	26.7
Fe_2O_3	81.7	28.0	76.6	26.2
SiO_2	112.8	38.6	76.6	26.2
CrO_3	162.7	58.5	76.6	27.6

Table 3-12

Coulomb Bond Energies Between R-CH_2 Si$(OH)_3$ and Various Oxides



Adsorbate: $R_S i(OH_2)$ Substrate Oxide	Dibasic U_M(kJ/mole)	U_N	Diacid U_M	U_N
Ag_2O	23.6	6.63	45.6	16.4
CuO	51.4	14.6	45.6	16.1
Fe_2O_3	77.0	21.8	45.6	15.9
SiO_2	106.0	30.0	45.6	15.9
CrO_3	153.2	45.6	45.6	16.7

Table 3-13

Bond Properties for Adsorbates and Substrate Oxides

Bond + - -	D_{AB} (kJ/mole)	%I	L_{AB}	μ (debye)	R_A	R_B
H - O	435	34.1	0.94	1.54	0.32	0.73
H - N	366	18.6	0.99	0.88	0.32	0.75
Cr = O	1051	58.2	1.64	4.58	1.18	0.62
Ag - O	362	60.9	1.93	5.64	1.34	0.73
Cu - O	384	59.5	1.76	5.03	1.17	0.73
Fe - O	421	59.4	1.76	4.56	1.17	0.73
Si - O	387	59.1	1.70	4.82	1.11	0.73
Cr - O	494	61.9	1.75	5.20	1.18	0.73
Si - C	303	13.4	1.82	1.17	1.11	0.77

Table 3-14

Comparison of Revised (Ref. 1 = X) and Pauling (Ref. 2 = X_p) Values of Elemental Electronegativity

AT. No.	SY	X	X_p	$X-X_p$	AT. No.	SY	X	X_p	$X-X_p$
1	H	2.20	2.1	0.10	37	RB	0.82	0.8	0.02
					38	SR	0.95	1.0	-0.05
3	LI	0.98	1.0	-0.02	38	Y	1.22	1.2	0.02
4	BE	1.57	1.5	0.07	40	ZR	1.33	1.4	-0.07
5	B	2.04	2.0	0.04	41	NB	1.60	1.6	0.0
6	C	2.55	2.5	0.05	42	MO	2.16	1.8	0.36
7	N	3.04	3.0	0.04	43	TC	1.90	1.9	0.0
8	O	3.44	3.5	-0.06	44	RU	2.20	2.2	0.0
9	F	3.98	4.0	-0.02	45	RH	2.28	2.2	0.08
					46	PD	2.20	2.2	0.0
11	NA	0.93	0.9	0.03	47	AG	1.93	1.9	0.03
12	MG	1.31	1.2	0.11	48	CD	1.69	1.7	-0.01
13	AL	1.61	1.5	0.11	49	IN	1.78	1.7	0.08
14	SI	1.90	1.8	0.10	50	SN	1.96	1.8	0.16
15	P	2.19	2.1	0.19	51	SB	2.05	1.9	0.15
16	S	2.58	2.5	0.08	52	TE	2.10	2.1	0.0
17	CL	3.16	3.0	0.16	53	I	2.66	2.5	0.16
19	K	0.82	0.8	0.02	55	CS	0.79	0.7	0.09
20	CA	1.00	1.0	0.0	56	BA	0.89	0.9	-0.01
21	SC	1.36	1.3	0.06	57	LA	1.10	1.1	0.0
22	TI	1.54	1.5	0.04	72	HF	1.30	1.3	0.0
23	V	1.63	1.6	0.03	73	TA	1.50	1.5	0.0
24	CR	1.66	1.6	0.06	74	W	2.36	1.7	0.66
25	MN	1.55	1.5	0.05	75	RE	1.90	1.9	0.0
26	FE	1.83	1.8	0.03	76	OS	2.20	2.2	0.0
27	CO	1.88	1.8	0.08	77	IR	2.20	2.2	0.0
28	NI	1.91	1.8	0.11	78	PT	2.28	2.2	0.08
29	CU	1.90	1.9	0.0	79	AU	2.54	2.4	0.14
30	ZN	1.65	1.6	0.05	80	HG	2.00	1.9	0.10
31	GA	1.81	1.6	0.21	81	TL	2.04	1.8	0.24
32	GE	2.01	1.8	0.21	82	PB	2.33	1.8	0.53
33	AS	2.18	2.0	0.18	83	BI	2.02	1.9	0.12
34	SE	2.55	2.4	0.15					
35	BR	2.96	2.8	0.16	90	TH	1.30	1.3	0.0
					92	U	1.38	1.7	-0.32
					94	PU	1.28	-	-

Table 4-1

Functional Group Properties for Polymers

Unit No.	(R = 8.314 J/K°mole) Structure Group	U (J/mole)	H	N	V (m^3/mole)	M (kg/mole)	Polymer Unit
1	-CH2-	6.14E3	8	1	2.22E-5	1.4E-2	ethylene
2	-CH(CH3)-	1.20E4	11	1	4.44E-5	2.8E-2	propylene
3	-C((CH3)2)-	1.19E4	14	1	6.66E-5	4.2E-2	isobutylene
4	-CH(C6H4)-	3.01E4	15	1	1.11E-4	9.0E-2	styrene
5	-P-C6H4-	2.30E4	5	4	8.86E-5	7.6E-2	terephthlate
6	-M-C6H4-	2.58E4	10	3	8.86E-5	7.6E-2	isophthalate
7	-C(CH3)CH-	1.15E4	11	2	5.92E-5	4.0E-2	isoprene
8	-CHCH-	7.49E3	8	2	3.70E-5	2.6E-2	1,4-butadiene
9	-CH(CHCH2)-	1.29E4	11	1	5.90E-5	4.0E-2	1,2-butadiene
10	-CH(C6H11)-	2.56E4	21	1	1.48E-4	9.6E-2	vinyl cyclohexane
11	-CH(C(O)OCH3)-	2.81E4	23	1	7.57E-5	7.2E-2	methacrylate
12	-C(CH3)(C(O)OCH3)-	4.60E4	26	1	9.79E-5	8.6E-2	methylmethacrylate
13	-CH(CH3)O-	1.39E4	17	2	5.54E-5	4.4E-2	propylene oxide
14	-C(O)O-	1.41E4	12	2	3.32E-5	4.4E-2	ethylene adipate
15	-CH(OC(O)CH3)-	3.17E4	23	1	7.57E-5	7.2E-2	vinyl acetate
16	-C(O)-	7.32E3	6	1	2.22E-5	2.8E-2	ketone
17	-CH(C(O)OH)-	3.51E4	20	1	5.64E-5	5.[illegible]E-2	acrylic acid
18	-CH(OH)-	2.66E4	14	1	4.90E-5	3.0E-2	vinyl alcohol
19	-CH(OCH(O))-	2.86E4	20	1	5.54E-5	5.[illegible]E-2	vinyl formate
20	-O-	6.82E3	6	1	1.06E-5	1.6E-2	ether
21	-NHC(O)-	4.44E4	13	2	3.79E-5	4.3E-2	amide
22	-NHC(O)O-	2.63E4	19	3	4.89E-5	5.9E-2	urethane
23	-CH(CN)-	2.41E4	8	1	4.89E-5	3.9E-2	acrylonitrile
24	-CH(CL)-	1.75E4	8	1	4.07E-5	4.85E-2	vinyl chloride
25	-C(CL)CH-	1.26E4	8	2	5.55E-5	6.05E-2	neoprene
26	-C((CL)2)-	1.13E4	8	1	5.92E-5	8.30E-2	vinylidene chloride
27	-CF2-	4.81E3	8	1	3.4[illegible]E-5	5.0E-2	tetrafluoroethylene
28	-CH2CF2-	1.48E4	16	2	5.70E-5	6.4E-2	vinylidene fluoride
29	-CF(CF3)-	1.84E4	13	1	6.96E-5	1.0E-1	perfluoropropylene
30	-SI((CH3)2)O-	1.72E4	30	2	8.62E-5	7.4E-2	dimethylsiloxane
31	-N((C(O))2)C6H2((C(O))2)N-	1.10E5	62	7	2.01E-4	2.14E-1	imide
32	-S-	8.26E3	8	1	2.56E-5	3.2E-2	sulfide
33	-S((O)2)	4.54E4	23	1	4.04E-5	6.40E-2	sulfone

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Table 4-2
Sample Computations for Methacrylates (Upper Case) and Butadiene-Styrene Copolymers (Lower Case)

Unit No.	Moles	Structure Unit	Polymer Reference
		I. Main Chain Units	
1	1	-CH2-	ethlyene
12	1	-C(CH3)(C(O))CH3)-	methyl methacrylate
		II. Side Chain Units	
1	11	-CH2-	ethylene
Glass Spec. Vol. (M*M*M/kg = 9.89634E-04 (CC/G) = 0.989634			
Glass C.E.D. (J/M*M*M) = 3.7802E+08 (CAL/CC) = 90.3904			
Glass Temp (K) = 214.007 (C) = -59.1928			
Entang. MW (kg/mole) = 88.7177 (g/mole) = 88717.7			
		I. Main Chain Units	
1	0.87	-CH2-	ethylene
8	0.87	-CHCH-	1,4-butadiene
1	0.87	-CH2-	ethylene
1	0.13	-CH2-	ethylene
4	0.13	-CH(C6H5)-	styrene
Glass Spec. Vol. (M*M*M/kg) = 1.00516E-03 (CC/G) = 1.00516			
Glass C.E.D. (J/M*M*M) = 2.96893E + 8 (CAL/CC) = 70.9575			
Glass Temp (K) = 208.462 (C) = -64.7382			
Entang. MW (kg/mole) = 2.58618 (g/mole) = 2586.18			

Table 4-3
Comparison of Calculated and Experimental T_g (Ref 2,4)

Methacrylates		V_p (g/cc)	δ^2 (cal/cc)	T_g (C)	M_e (kg/mole)	T_g (exp) (C)
methyl		0.829	144	107	18.2	105
ethyl		0.861	131	63	23.1	61
propyl		0.886	122	33	28.4	31
butyl		0.907	115	12	34.0	12
hexyl		0.938	105	-17	46.1	-19
octyl		0.989	90	-36	59.3	-38
dodecyl		0.989	90	-59	88.7	-62
Butadiene-Styrene Copolymers						
Mole (B)	Mole (S)					
0	1	0.883	88	110	20.2	100
0.2	0.8	0.902	86	69	12.8	-
0.4	0.6	0.923	82	28	8.2	-
0.61	0.39	0.954	77	-14	5.0	-12
0.64	0.36	0.959	77	-20	4.7	-13
0.72	0.28	0.973	75	-35	3.9	-34
0.77	0.23	0.983	74	-45	3.4	-37
0.87	0.13	1.01	71	-64	2.6	-51,-60
0.95	0.05	1.03	68	-80	2.0	-71,-76
0.99	0.01	1.04	67	-88	1.8	-74
1.00	0	1.04	67	-90	1.7	-79,-87

Table 4-4
Calculated and Experimental Values of M_e

Polymer	M_e (kg/mole)	M_e (exp) (kg/mole)
poly-n-octylmethacrylate	59.3	87
poly-n-hexylmethacrylate	46.1	33.9
polymethylmethacrylate	18.2	4.7-10.0
polystyrene	20.2	17.3-18.1
styrene-butadiene copolymer (0.87 mole St, o.13 mole Bd)	2.6	3.0
poly-1,4-polybutadiene	1.7	1.7-2.9

Table 4-5
Relation of Stress-Strain Curve Number to Test Temperature

Curve No.	Temp (K)	Curve No.	Temp (K)	Curve No.	Temp (K)
1	180	8	285	15	390
2	195	9	300	16	405
3	210	10	315	17	420
4	225	11	330	18	435
5	240	12	345	19	450
6	255	13	360	20	465
7	270	14	375	21	480

Table 4-6
Functional Group Properties for Polymers

Structure Group	U (J/mole)	B	N	V (m^3/mole)	M (kg/mole)	Reference Polymer
-M-C6H4-	2.58E4	10	3	8.86E-5	7.6E-2	isophthalate
-P-C6H4-	2.38E4	5	4	8.86E-5	7.6E-2	terepthalate
-O-	6.82E3	6	1	1.06E-5	1.6E-2	ether
-CHCH-	7.49E3	8	2	3.70E-5	2.6E-2	1, 4-butadiene
-S((O)2)-	4.54E4	23	1	4.04E-5	6.4E-2	sulfone

Table 4-7
Computed Estimates of ATS Physical Properties from Chemical Structure

Unit No.	Moles	Structures Unit	Polymer Reference
6	2	-M-C6H4	Isophthalate
5	2	-P-C6H4	Terephthalate
20	2	-O-	Ether
8	2	-CHCH-	1-4-Butadiene
33	1	-S((0)2)-	Sulfone

Glass Spec. Vol (M*M*M/KG) = 7 48009E-04 (CC/G) = .748009
Glass C.E.O. (J/M*M*M) = 5.09055E+08 (CAL/CC) = 121.664
Glass Temp. (K) 540.383 (C) = 267.183
Entang. M (KG/Mole) = 3.39525 (G/MOLE) = 3395.25
U,H,V,M,N 173220 81 4.9E-04 452 21 (Summed Values)

Table 4-8
Relation of Stress-Strain Curve Number to Test Temperature at Constant Time t = 1.0 s

Curve No.	Temperature °C	Temperature K	Curve No.	Temperature °C	Temperature K
1	-50	223	11	200	473
2	-25	248	12	225	498
3	0	273	13	250	523
4	25	248	14	275	548
5	50	323	15	300	573
6	75	348	16	325	598
7	100	373	17	350	623
8	125	398	18	375	648
9	150	423	19	400	673
10	175	448			

Table 5-1
Properties of Commercial Reinforcing Fibers
(from Ref. 5, p. 47)

Fiber	Spec. Vol. (cc/g)	Tensile Properties			
		E (GPa)	S_b (GPa)	ϵ_b (%)	W_b (MPa)
Graphite (UHM-S)	0.510	500	1.86	0.37	3.44
(HM-S)	0.523	360	2.34	0.65	7.60
(HT-S)	0.565	244	2.82	1.16	16.36
(A-S)	0.571	208	2.82	1.36	19.18
Boron (W-core)	0.377	386	3.41	0.88	15.00
Aramid-49	0.690	138	2.76	2.00	27.60
E-glass	0.394	72.5	3.44	4.74	81.53

Table 5-2

Estimated Elemental Properties of Carbon

```
HOW MANY ELEMENTS? 1
ELEMENT CODE NO =? 5
MOLES OF ELEMENT=? 2
NUMBER OF CHEMICAL BOND TYPES=? 1
FOR A-B BOND, ELEMENT A CODE NO =? 5
ELEMENT B CODE NO =? 5
MOLES OF A-B BONDS=? 4_


ELEMENTARY PROPERTIES
Z, SY, W, D/1E5, X, R/1E-10, V  PH =
 6 C 12.01  3.42  2.55   77  4  5
TO CONTINUE PRESS ENTER
?
CHEMICAL ANALYSIS:

BONDING          BOND       % IONIC   BOND       MOLES
ELEMENTS         ENERGY     ENERGY    LENGTH
A     B          (J/MOLE)             (M*1E-10)
C     C           348030     0         1.54        4
TOTAL             1.392E+06                        4
TO CONTINUE PRESS ENTER
?
PHYSICAL ANALYSIS:
ELEMENTS         MOLES
C                 2
MOLECULAR WT. (KG/MOLE)= .02402
                 MOLE)= 24.02
SPECIF.  VOLUM    /G) :
(Z=12)           Z=8)          (Z=6)          Z=4)
 .129547          .140348       .18313         .232413
TO CONTINUE T    RUN AND PRESS ENTER
READY
>_
```

Table 5-3

Estimated Intramolecular Properties of Silica

```
HOW MANY ELEMENTS? 2
ELEMENT CODE NO =? 12
MOLES OF ELEMENT=? 1
ELEMENT CODE NO =? 7
MOLES OF ELEMENT=? 2
NUMBER OF CHEMICAL BOND TYPES=? 1
FOR A-B BOND, ELEMENT A CODE NO =? 12
ELEMENT B CODE NO =? 7
MOLES OF A-B BONDS=? 4_

ELEMENTARY PROPERTIES
Z, SY, W, D/1E5, X, R/1E-10, V, PH =
 14 SI 28 09 : 1.77  1 9  1 11  4  7
 8 O 16  1.39  3.44   73  2  2
TO CONTINUE PRESS ENTER
?
CHEMICAL ANALYSIS:

BONDING            BOND        % IONIC    BOND         MOLES
ELEMENTS           ENERGY      ENERGY     LENGTH
A      B           (J/MOLE)               (M*1E-10)
SI     O           386960      59.1583    1.7014       4
TOTAL              1.54744E+06                         4
TO CONTINUE PRESS ENTER
?
PHYSICAL ANALYSIS:
ELEMENTS           MOLES
SI                 1
O                  2
MOLECULAR WT. (KG/MOLE)= .06009
                 (G/MOLE)= 60.09
SPECIFIC VOLUME (CC/G) :
(Z=12)              (Z=8)              (Z=6)              (Z=4)
 .104749             .113966            .148114            .228352
TO CONTINUE TYPE RUN AND PRESS ENTER
READY
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```

Table 5-4

Estimated Intramolecular Properties of Aramid

```
HOW MANY ELEMENTS? 4
ELEMENT CODE NO.=? 1
MOLES OF ELEMENT=? 5
ELEMENT CODE NO =? 5
MOLES OF ELEMENT=? 7
ELEMENT CODE NO.=? 6
MOLES OF ELEMENT=? 1
ELEMENT CODE NO.=? 7
MOLES OF ELEMENT=? 1
NUMBER OF CHEMICAL BOND TYPES=? 2
FOR A-B BOND, ELEMENT A CODE NO.=? 5
ELEMENT B CODE NO.=? 5
MOLES OF A-B BONDS=? 10
FOR A-B BOND, ELEMENT A CODE NO.=? 6
ELEMENT B CODE NO =? 5
MOLES OF A-B BONDS=? 2_


 1 H 1.008  4.35  2.2   .32  1  7
 6 C 12.01  3.48  2.55  .77  4  5
 7 N 14.01  1 61  3.04  75  3  2
 8 O 16  1.39  3.44  .73  2  2
TO CONTINUE PRESS ENTER
?
CHEMICAL ANALYSIS:

BONDING            BOND        % IONIC     BOND         MOLES
ELEMENTS           ENERGY      ENERGY      LENGTH
A     B            (J/MOLE)                (M*1E-10)
C     C             348000      0           1.54         10
N     C             277670      8.34433     1.4759       2
TOTAL               4.83534E+06                          12


TO CONTINUE PRESS ENTER
?
PHYSICAL ANALYSIS:
ELEMENTS           MOLES
H                   5
C                   7
N                   1
O                   1
MOLECULAR WT. (KG/MOLE)= .11912
              (G/MOLE)= 119.12
SPECIFIC VOLUME (CC/G):
(Z=12)             (Z=8)              (Z=6)              (Z=4)
  179209           .194979            .253402            .390675
TO CONTINUE TYPE RUN AND PRESS ENTER
READY
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```

Table 5-5

Calculated Specific Bond Energy for Fibers
(Chemical energy/unit mass)

Fibers	Molar Composition	Molar of Bonds	Total Bond Energy (J/mol)	Mol. Wt. (g/mol)	Spec. Bond Energy (J/g)
Commercial					
Carbon	(C_2)	4	1.39E6	24.02	5.79E4
Boron	(B_2)	3	7.59E6	21.62	3.51E4
Aramid-49		12	4.04E6	119.1	3.39E4
Alumina	(Al_2O_3)	6	2.97E6	102.0	2.91E4
Silica	(SiO_2)	4	1.55E6	60.1	2.58E4
Aluminum	(Al_2)	3	6.18E5	53.96	1.15E4
Titanium	$(Ti)_2$	4	1.06E6	95.8	1.11E4
Iron	(Fe_2)	3	6.09E5	111.7	5.45E3
Candidates					
Boron Nitride	$(B_{12}N_5)$	3	9.11E5	24.82	3.67E4
Silicon Carbide	(SiC)	4	1.21E6	40.1	3.02E4
Polyethylene	$(-CH_2-)$	1	3.48E5	14.0	2.48E4
Carbon Precursor					
PAN	$[CH_2-CH(CN)]$	2	6.96E5	51.1	1.36E4

Table 5-6

Estimated Physical Properties of Equimolar TGMDA and DDS Linear Polymer (see Fig. 5-3)

```
MONOMER-POLYMER PREDICTION PART-1,D.H KAELBLE MAY,81
HOW MANY MAIN CHAIN UNITS?? 6
STRUCTURE UNIT NO =? 5
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO =? 33
MOLES OF STRUCTURE UNIT=? 1
STRUCTURE UNIT NO =? 1
MOLES OF STRUCTURE UNIT=? 5
STRUCTURE UNIT NO =? 18
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO =? 21
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO =? 16
MOLES OF STRUCTURE UNIT=? -4
HOW MANY SIDE GROUPS? (NONE=0)? 3
STRUCTURE UNIT NO.=? 1
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO =? 8
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO =? 20
MOLES OF STRUCTURE UNIT=? 2


I. MAIN CHAIN UNITS
UNIT NO. MOLES STRUCTURE                      POLYMER
               UNIT                           REFERENCE
 5        4    -P-C6H4-                       TEREPHTHALATE
 33       1    -S((O)2)-                      SULFONE
 1        5    -CH2-                          ETHYLENE
 18       2    -CH(OH)-                       VINYL ALCOHOL
 21       4    -NHC(O)-                       AMIDE
 16      -4    -C(O)-                         KETONE
II  SIDE CHAIN UNITS
 1        2    -CH2-                          ETHYLENE
 8        2    -CHCH-                         1-4-BUTADIENE
 20       2    -O-                            ETHER
GLASS SPEC. VOL (M*M*M/KG)=  8.30266E-04 (CC/G)= .830266
GLASS C.E.D. (J/M*M*M)=  7.13963E+08 (CAL/CC)= 170.637
GLASS TEMP. (K)=  551.407 (C)= 273.207
ENTANG. MW. (KG/MOLE)=  4.33352 (G/MOLE)= 4833.52
U,H,V,M,N 399720  183  8.052E-04  .67  28
TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>_
```

Table 5-7

Estimated Physical Properties of 2 Moles of TGMDA and
1 Mole of DDS Linear Polymer (see Fig. 5-4)

```
MONOMER-POLYMER PREDICTION PART-1,D H KAELBLE MAY,81
HOW MANY MAIN CHAIN UNITS?? 6
STRUCTURE UNIT NO =? 5
MOLES OF STRUCTURE UNIT=? 6
STRUCTURE UNIT NO.=? 33
MOLES OF STRUCTURE UNIT=? 1
STRUCTURE UNIT NO.=? 1
MOLES OF STRUCTURE UNIT=? 10
STRUCTURE UNIT NO.=? 19
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO.=? 21
MOLES OF STRUCTURE UNIT=? 6
STRUCTURE UNIT NO.=? 16
MOLES OF STRUCTURE UNIT=? -6
HOW MANY SIDE GROUPS? (NONE=0)? 3
STRUCTURE UNIT NO.=? 1
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO.=? 8
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO.=? 20
MOLES OF STRUCTURE UNIT=? 4_

I. MAIN CHAIN UNITS
UNIT NO. MOLES STRUCTURE                          POLYMER
               UNIT                               REFERENCE
 5        6    -P-C6H4-                           TEREPHTHALATE
 33       1    -S((O)2)-                          SULFONE
 1        10   -CH2-                              ETHYLENE
 18       4    -CH(OH)-                           VINYL ALCOHOL
 21       6    -NHC(O)-                           AMIDE
 16      -6    -C(O)-                             KETONE
II. SIDE CHAIN UNITS:
 1        4    -CH2-                              ETHYLENE
 8        4    -CHCH-                             1-4-BUTADIENE
 20       4    -O-                                ETHER
GLASS SPEC. VOL.(M*M*M/KG)=  0.59914E-04 (CC/G)= .859914
GLASS C.E D .(J/M*M*M)=  6.67803E+08 (CAL/CC)= 159 605
GLASS TEMP. (K)=  502.679 (C)= 229.479
ENTANG. MW. (KG/MOLE)=  5 15813 (G/MOLE)= 5168 13
U,H,V,X,N 632200 .319  1 3634E-03  1 094  45
TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>_
```

Table 5-8

Estimated Physical Properties of TGMDA Linear Homopolymer (see Fig. 5-5)

```
MONOMER-POLYMER PREDICTION PART-1 D.H KAELBLE MAY,81
HOW MANY MAIN CHAIN UNITS?? 5
STRUCTURE UNIT NO =? 5
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO.=? 1
MOLES OF STRUCTURE UNIT=? 5
STRUCTURE UNIT NO =? 8
MOLES OF STRUCTURE UNIT=? 1
STRUCTURE UNIT NO.=? 21
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO.=? 16
MOLES OF STRUCTURE UNIT=? -2
HOW MANY SIDE GROUPS? (NONE=0)? 3
STRUCTURE UNIT NO =? 20
MOLES OF STRUCTURE UNIT=? 4
STRUCTURE UNIT NO =? 1
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO.=? 8
MOLES OF STRUCTURE UNIT=? 2_

I. MAIN CHAIN UNITS:
UNIT NO. MOLES STRUCTURE                                  POLYMER
               UNIT                                       REFERENCE
 5        2    -P-C6H4-                                   TEREPHTHALATE
 1        5    -CH2-                                      ETHYLENE
 8        1    -CHCH-                                     1-4-BUTADIENE
 21       2    -NHC(O)-                                   AMIDE
 16      -2    -C(O)-                                     KETONE
II. SIDE CHAIN UNITS:
 20       4    -O-                                        ETHER
 1        2    -CH2-                                      ETHYLENE
 8        2    -CHCH-                                     1-4-BUTADIENE
GLASS SPEC. VOL.(M*M*M/KG)=  8.45986E-04 (CC/G)= .845986
GLASS C.E.D. (J/M*M*M)=  5.57993E+08 (CAL/CC)= 133.36
GLASS TEMP. (K)=  402.405 (C)= 129.295
ENTANG. MW. (KG/MOLE)=  5.30042 (G/MOLE)= 5300.42
U,M,V,M,N 200490  128  5.174E-04  .422  17
TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>_
```

Table 5-9

First Estimate of the Physical Properties of Equimolar Isoamyl-Neopentyl Acrylate Copolymer

```
MONOMER-POLYMER PREDICTION PART-1.D.H.KAELBLE MAY,81
HOW MANY MAIN CHAIN UNITS?? 1
STRUCTURE UNIT NO.=? 1
MOLES OF STRUCTURE UNIT=? 4
HOW MANY SIDE GROUPS? (NONE=0)? 4
STRUCTURE UNIT NO.=? 14
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO.=? 1
MOLES OF STRUCTURE UNIT=? 5
STRUCTURE UNIT NO.=? 2
MOLES OF STRUCTURE UNIT=? 1
STRUCTURE UNIT NO.=? 3
MOLES OF STRUCTURE UNIT=? 1_


UNIT NO.  MOLES STRUCTURE                          POLYMER
                UNIT                               REFERENCE
 1         4    -CH2-                              ETHYLENE
II. SIDE CHAIN UNITS:
 14        2    -C(O)O-                            ETHYLENE ADIPATE
 1         5    -CH2-                              ETHYLENE
 2         1    -CH(CH3)-                          PROPYLENE
 3         1    -C((CH3)2)-                        ISOBUTYLENE
GLASS SPEC. VOL.(M*M*M/KG)=  9.16437E-04 (CC/G)= .916437
GLASS C.E.D. (J/M*M*M)=  3.44195E+08 (CAL/CC)= 82.2626
GLASS TEMP. (K)=  204.375 (C)=-68.6251
ENTANG. MW. (KG/MOLE)=  34.185 (G/MOLE)= 34185
U,H,V,M,N 90160  121  3.772E-04   284  4
TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>_
```

Table 5-10

Second Estimate of the Physical Properties of Equimolar Isoamyl-Neopentyl Acrylate Copolymer

```
MONOMER-POLYMER PREDICTION PART-1,D H KAELBLE MAY,81
HOW MANY MAIN CHAIN UNITS?? 2
STRUCTURE UNIT NO =? 1
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO =? 2
MOLES OF STRUCTURE UNIT=? 2
HOW MANY SIDE GROUPS? (NONE=0)? 4
STRUCTURE UNIT NO =? 14
MOLES OF STRUCTURE UNIT=? 2
STRUCTURE UNIT NO =? 1
MOLES OF STRUCTURE UNIT=? 3
STRUCTURE UNIT NO =? 2
MOLES OF STRUCTURE UNIT=? 1
STRUCTURE UNIT NO =? 3
MOLES OF STRUCTURE UNIT=? 1

I. MAIN CHAIN UNITS:
UNIT NO. MOLES STRUCTURE                          POLYMER
               UNIT                               REFERENCE
 1       2     -CH2-                              ETHYLENE
 2       2     -CH(CH3)-                          PROPYLENE
II. SIDE CHAIN UNITS:
 14      2     -C(O)O-                            ETHYLENE ADIPATE
 1       3     -CH2-                              ETHYLENE
 2       1     -CH(CH3)-                          PROPYLENE
 3       1     -C((CH3)2)-                        ISOBUTYLENE
GLASS SPEC. VOL.(M*M*M/KG)=  9.16437E-04 (CC/G)=  .916437
GLASS C.E.D. (J/M*M*M)=  3.78786E+08 (CAL/CC)= 90.5189
GLASS TEMP. (K)=  240.38 (C)=-32.8198
ENTANG. MW. (KG/MOLE)=  34.185 (G/MOLE)= 34185
U,H,V,M,N 99208  111  3.772E-04   284  4
TO CONTINUE TYPE RUN AND PRESS ENTER
READY
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Table 5-11

Relations Between Polymer Chemistry and Physical Properties

Polymer Number	Polymer	Calc. V_s $(\frac{cc}{g})$	Calc. δ^2 $(\frac{cal}{cc})$	Calc. T_g (K)	Calc. M_e $(\frac{kg}{mol})$	Exp.[18] M_e $(\frac{kg}{mol})$
1	p-dimethyl siloxane	0.81	68.7	163	10.6	12.2
2	p-isobutylene	1.09	62.1	201	8.2	8.0
3	p-cisisoprene	1.05	65.7	201	3.1	3.8
4	p-cis-transbutadiene	1.04	66.7	183	1.7	2.2
5	p-cisbutadiene	1.04	66.7	183	1.7	3.0
6	p-ethylene	1.09	64.2	150	2.1	2.5
7	p-propylene	1.09	87.5	240	4.9	3.5
8	p-styrene	0.88	88.5	384	20.2	17.5
9	p-α-methyl styrene	0.91	90.3	434	25.2	20.4
10	p-ethyleneoxide	0.86	94.5	190	1.5	3.0
11	p-propyleneoxide	0.92	105.9	254	3.5	3.9
12	p-tetramethylene oxide	0.95	81.0	173	1.8	1.3
13	p-methylacrylate	0.79	113.3	276	13.6	12.1
14	p-methylmethacrylate	0.83	143.7	380	18.1	15.8
15	p-n-butylmethacrylate	0.91	115.3	285	34.0	30.2
16	p-n-hexylmethacrylate	0.94	105.4	256	46.1	45.9
17	p-n-octylmethacrylate	0.96	98.8	237	59.3	57.0
18	p-2 ethylbutylmethacrylate	0.94	112.2	288	46.1	21.4
19	p-vinylacetate	0.79	125.9	304	13.6	12.3
20	p-vinylalchohol	1.12	148.6	362	5.4	3.8
21	p-vinylchloride	0.69	118.4	351	6.9	3.2
22	p-decamethyleneadipate	0.92	78.6	177	2.1	2.2
23	p-decamethylenesebecate	0.95	75.8	172	2.1	2.4
24	p-decamethylenesuccinate	0.90	80.5	181	2.1	2.3
25	p-ethyleneterephthalate	0.72	104.0	348	2.4	1.7
26	p-ethyleneisophthalate	0.72	104.0	348	2.4	1.7
27	p-bisphenol-A-carbonate	0.70	96.4	400	3.5	2.5
28	p-bisphenol-A-diphenyl-sulfone	0.75	118.4	533	3.6	3.6
29	p-2-methyl-6 phenyl-1,4-phenylene oxide	0.80	96.0	613	10.3	1.7
30	p-2, 6-dimethyl-1, 4-phenylene oxide	0.83	93.2	501	4.8	1.7
31	p-caprolactam	0.91	150.5	321	2.2	2.5
32	p-propylene sulfide	0.87	93.1	250	5.4	10.0
33	p-acrylic acid	0.75	171.8	363	9.6	2.4
34	p-acrylonitrile	0.93	136.7	450	6.5	0.65
35	p-tetrafluoroethylene	0.48	47.6	169	12.0	6.6
36	p-acrylamide	0.80	220.3	463	9.8	4.6
37	p-phenyleneterephthalamide	0.73	185.5	938	2.7	0.6
38	p-benzamide	0.73	185.5	938	2.7	0.4
39	p-n-hexylisocyanate	0.93	139.2	299	28.8	3.7
40	p-n-butylisocyanate	0.88	165.5	351	18.6	0.35

Table 5-12

Summed Properties of Functional Groups

Polymer Number	U $(\frac{J}{mol})$	H	V $(\frac{cc}{mol})$	M $(\frac{g}{mol})$	N	$-(\frac{\partial\sigma_{12}}{\partial T})_g$ $(\frac{bar}{deg})$	Shear Yield σ_{12} (at 293K) bar
1	17200	30	86.2	74	2	9.9	0
2	16040	22	88.8	56	2	7.0	0
3	19780	27	103.6	68	4	7.4	0
4	15770	24	81.4	54	4	8.3	0
5	15770	24	81.4	54	4	8.3	0
6	4140	8	22.2	14	1	10.2	0
7	16940	19	66.6	42	2	8.0	0
8	34240	23	133.0	104	2	4.9	446
9	40740	24	155.0	118	2	5.7	804
10	15100	22	55.0	44	3	11.3	0
11	23760	25	77.2	53	3	9.1	0
12	23380	30	99.4	72	5	11.1	0
13	32240	31	97.9	86	2	8.9	0
14	50140	34	120.1	100	2	8.0	696
15	62560	58	186.7	142	2	8.8	0
16	70840	74	231.1	170	2	9.1	0
17	79120	90	275.5	198	2	9.2	0
18	75360	60	231.1	170	2	8.4	0
19	35840	31	97.9	86	2	8.9	98
20	30740	22	71.2	44	2	8.7	600
21	21640	16	62.9	62.5	2	7.2	418
22	86160	136	377.2	284	18	10.2	0
23	102720	168	466.0	340	22	10.2	0
24	77280	120	332.8	256	16	10.2	0
25	60280	45	199.4	192	10	6.4	352
26	62280	50	199.4	192	9	7.1	227
27	80980	52	287.2	254	12	5.1	546
28	166660	79	482.6	442	20	4.6	1104
29	58560	24	210.0	182	5	3.3	947
30	43420	22	143.6	120	5	5.3	1102
31	65100	53	148.9	113	7	10.1	283
32	25200	27	93.1	74	3	8.2	0
33	39240	28	78.6	72	2	9.7	679
34	28240	16	71.1	53	2	6.4	1005
35	4810	8	34.8	50	1	9.9	0
36	52680	29	82.3	71	2	6.5	1105
37	68200	18	126.5	119	6	4.03	2599
38	68200	18	126.5	119	6	4.03	2599
39	69240	61	171.1	127	2	10.1	61
40	60960	45	126.7	99	2	8.5	493

Table 5-13

Polymerized Silane Chemistry and Surface Properties[19,20]

Test Liquid				H_2O	Glycerol	Eth. Glycol	PG E-200	PG 15-200	PB 1200
γ_{LV} (dyn/cm)				7.28	64.0	48.3	43.5	36.6	31.3
$2a_L$ (dyn/cm)$^{1/2}$				9.34	12.16	10.70	10.62	10.20	9.90
β_L/α_L				1.54	0.94	0.81	0.74	0.64	0.53
R-Structure	Source	γ_{SV}^d dyn/cm	γ_{SV}^p dyn/cm	$W_{SL}/2a_L$ (dyn/cm)$^{1/2}$					
$H_2N(CH_2)_2NH(CH_2)_3$-	DC Z-6020	30.0	4.6		7.54	7.21	6.99	6.92	
$CH_2{=}C(CH_3){-}C({=}O){-}O{-}(CH_2)_3$-	DC Z-6030	8.4	41.7		9.08	8.03	7.41	7.42	6.21
$\overset{O}{CH_2{-}CH}{-}CH_2O(CH_2)_3$- (catalyzed)	DC Z-6040	10.2	43.6	13.23	9.69	8.57	8.13	7.12	
$\overset{O}{CH_2{-}CH}{-}CH_2{-}O{-}(CH_2)_3$- (noncatalyzed)	DC Z-6040	17.6	25.4	11.94	9.01	8.29	7.87		
$Cl{-}(CH_2)_3$-	DC XZ-8-0999	36.5	3.8	9.09	7.80	7.21	7.90		
$NH_2{-}(CH_2{-})_3$	UC A-1100	17.9	19.8	11.35	7.63	7.76	7.41	7.63	
$HS{-}(CH_2{-})_3$	DC XZ-8-0951	67.4	0.0		8.06	8.33	8.02		
$CH_2{=}CH$-		28.5	2.1	7.72	6.25	6.35	6.56	6.81	5.90

Analysis of vapor-liquid-solid interactions for polymerized coatings of reactive silane coupling agents with structure $R{-}S_i(OCH_3)_3$.

Table 5-14
Reactive Silane Monomers[19,20]

Number	Reactive Silane
41	(dimethyl)(dimethoxy)silane - model compound
42	tetraethoxy silane
43	(vinyl)(triethoxy)silane
44	(γ-chloropropyl)(trimethoxy)silane
45	(γ-mercaptogropyl)(trimethoxy)silane
46	(methacryloxypropyl)(trimethoxy)silane
47	(γ-glycidoxypropyl)(trimethoxy)silane
48	(β-3, 4-epoxycyclohexylethyl)(trimethoxy)silane
49	(γ-aminopropyl)(trimethoxy)silane
50	(γ-aminopropyl)(trimethoxy)silane
51	N-β-aminoethyl-γ-aminopropyl(trimethoxy)silane
52	(4-styryl-methylene-β-aminoethyl-γ-aminopropyl)(trimethoxy)silane

Table 5-15

Linear Hydroxy Polymers of Reactive Silane Primers

Number	Linear Polymer
41	(dimethyl)siloxane
42	(dihydroxy)siloxane
43	(vinyl)(hydroxy)siloxane
44	(γ-chloropropyl)(hydroxy)siloxane
45	(γ-mercaptogropyl)(hydroxy)siloxane
46	(methacryloxypropyl)(hydroxy)siloxane
47	(γ-glycidoxypropyl)(hydroxy)siloxane
48	(β-3, 4-epoxycyclohexylethyl)(hydroxy)siloxane
49	(γ-aminopropyl)(hydroxy)siloxane
50	(γ-aminopropyl)(hydroxy)siloxane
51	N-β-aminoethyl-γ-aminopropyl(hydroxy)siloxane
52	(4-styryl-methylene-β-aminoethyl-γ-aminopropyl)(hydroxy)siloxane

Table 5-16

Summed Values of Monomer Group Properties for Lienar Hydroxy Polymers of Reactive Silane Primers

Number	U J/mole	H	V (cc/mole)	M	N
41	17200	30	86.2	74	2
42	44800	36	95.4	78	2
43	34350	33	105.6	88	2
44	52640	49	153.7	138.5	2
45	47540	57	161.7	136	2
46	66280	72	227.4	188	2
47	64550	77	215.6	176	2
48	62630	52	242	186	2
49	76360	56	151	119	2
50	76360	56	151	119	2
51	121720	79	211	162	2
52	157150	100	359	278	2

Table 5-17

Calculated Properties of Linear Hydroxy Polymers of Reactive Silanes at T_g

Number	V_s (cc/g)	δ^2 (cal/cc)	T_g (K)	M_e (kg/mole)
41	0.80	69	163	10.6
42	0.84	162	325	12.1
43	0.83	112	276	14.6
44	0.77	118	284	29.4
45	0.82	101	226	29.8
46	0.83	100	246	50.5
47	0.85	103	227	45.8
48	0.90	89	315	51.8
49	0.87	174	354	25.0
50	0.87	174	354	25.0
51	0.90	198	396	41.7
52	0.89	151	404	96.3

Table 5-18

Correlation Between Crosslink Density (ρ/M_c) and Maximum Network Extensibility $\lambda_b(max) = K(M_c/\rho)^{1/2}$

Polymer	T_g (°C)	$(M_c/\rho)^{1/2}$ $(cc/mole)^{1/2}$	$\lambda_b(max)$	K	Ref.
Silicone elastomer	-123	153	6.85	0.045	28
SBR elastomer	-61	113	7.20	0.064	28
Polybutadiene	-86	112	5.09	0.045	28
EPR elastomer	-55	105	6.85	0.065	28
Butyl elastomer	-70	104	6.17	0.059	28
Viton - b elastomer		93	5.19	0.056	28
Butyl elastomer	-70	92	7.20	0.078	28
Epoxy thermosett	115	31	1.59	0 051	28
Epoxy thermosett	72	23.2	1.27	0.055	29
Epoxy - polyamide	45	34.6	1.46	0.042	29
Epoxy - polyamide	20	56.4	1.95	0.035	29
Epoxy - polyamide	6	72	2.50	0.035	29
Viton - B elastomer		466	19.10	0.041	30
Viton - B elastomer		245	15.5	0.063	30
Viton - B elastomer		187	12.6	0.067	30
Viton - B elastomer		143	8.9	0.062	30
Viton - B elastomer		128	7.9	0.062	30
Viton - B elastomer		92	5.7	0.062	30
Epoxy - CTBN (50%)	-50	52.4	2.78	0.053	31
Epoxy - CTBN (39%)		47.0	2.41	0.051	31
Epoxy - CTBN (29%)		34.6	1.56	0.045	31
Epoxy - CTBN (17%)		30.6	1.32	0.044	31
Epoxy	100	29.2	1.35	0.046	31
			Ave. =	0.0515	
			Std. dev. =	±0.0150	

Table 5-19

Correlation Between Entanglement Crosslink Density (ρ/M_e) and Maximum Craze Extensibility $\lambda_c = K_c \cdot (M_e/\rho)^{1/2}$

Polymer	M_e (gm/mole)	$(M_e/\rho)^{1/2}$	λ_c	K_c
p-tert.-butylstyrene	4.3E4	203	7.2	0.035
p-para vinyltoluene	2.5E4	151	4.5	0.030
p-styrene	1.9E4	129	3.8	0.029
p-styrene-maleicanhydride (9 wt%)	1.9E4	128	4.2	0.033
p-styrene-acrylonitrile (24 wt%)	1.2E4	103	2.7	0.026
p-methylmethacrylate	9.2E3	87	2.0	0.023
p-styrene-methylmethacrylate (65 wt%)	9.0E3	87	2.0	0.023
p-styrene-acrylonitrile (66 wt%)	6.4E3	76	2.0	0.026
p-2,6 dimethyl-1,4-phenylene oxide (-E)	4.3E3	60	2.6	0.043
p-2,6 dimethyl-1,4-phenylene oxide (-M)	7.4E3	78	2.6	0.033
p-bisphenol-A carbonate	2.5E3	42	2.0	0.048
			Ave. =	0.032
			Std. Dev. =	±0.008

Note: M_e and λ_c data generated by experiments of Donald and Kramer (Ref. 7) and ρ is calculated from molecular structure.

Table 5-20
Correlation of Polymer Cohesive Energy δ_p^2 Density and Maximum Tensile Strength $(\sigma_{11})_b$ at 80 to 130K

	Chemical Composition	Calc. δ_p^2 (bar)	Meas. $(\sigma_{11})_b$ (bar)	$(\sigma_{11})_b/\delta_p^2$
1)	Fluorocopolymer $(C_2F_4)_{1.0}$ $(C_3F_6)_{0.136}$	1667	980	0.59
2)	C_2F_4 Homopolymer	1735	794	0.46
3)	Fluorocopolymer $(CF_2CFCl)_{1.0}(CF_2CH_2)_{0.031}$	2608	1147	0.44
4)	Bisphenol-A Carbonate $(OC_6H_4C(CH_3)_2C_6H_4OC(O))$	4088	1333	0.33
5	Polyethylene Terephthalate	5225	2108	0.40
6	Polyimide $(N(CO)_2C_6H_2(CO_2)NC_6H_4OC_6H_4)$	6186	2157	0.35
	Average			0.43
	Standard dev. ±			0.09

Table 5-21

Estimated Cure Path Properties of Equimolar TGMDA and DDS (see Table 5-6)

A AND B COREACTION-MOL. WT. DIST -THERMAL TRANS -D.H.KAELBLE-OCT. 27,1982
IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS
MOLES OF TYPE A (MOLE)=? 1
TYPE A FUNTIONALITY(=>2)=? 4
MOL. WT. OF TYPE A (G/MOLE)=? 248
MOLES OF TYPE B (MOLE)=? 1
TYPE B FUNCTIONALITY (=>2)=? 4
MOL. WT. OF TYPE B (G/MOLE)=? 422
FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 1
NUMBER OF A AND B MAIN CHAIN ATOMS (A1 A2)=? 11 17
MOL. WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 4833
GLASS COORDINATION NUMBER (8<Z<10)=? 10
MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T1,T2) IN DEG. K=
? 260,551
GEL POINT (% A REACTED)= 33.3333
GEL POINT (% B REACTED)= 33.3333
INITIAL NUM. AVE. DEG. OF POLYMERIZATION= 2.23368
TO ANALYSE POLYMERIZATION PRESS ENTER?

% A REACTED	BRANCH COEF	NUM. AVE. MW(G/MOL)	WT. AVE MW(G/MOL)	GLASS TEMP(K)	FLOW TEMP(K)
0	0	335	335	260	267.829
3.32667	.0332667	358.877	384.519	269.469	277.773
6.65334	.0665334	386.42	446.388	279.653	288.48
9.98001	.0998001	418.541	525.082	290.638	300.049
13.3067	.133067	456.486	631.787	302.52	312.539
16.6333	.166333	501.998	779.984	315.416	325.28
19.96	.1996	557.59	1001.66	329.46	341.283
23.2867	.232267	627.029	1370.31	344.313	357.83
26.6134	.266134	716.221	2103.95	361.567	376.516
29.94	.2994	934.995	4276.06	380.253	398.276
33.2667	.332667	1001	223324	408.353	491.121

TO ANALYSE CROSSLINKING PRESS ENTER? _

%A REACTED	BRANCH COEF	WT. FR. GEL	NUM AVE MW(G/MOL)	X-LINK MW (G/MOL)	GLASS TEMP(K)
33.4169	.334169	.0100001	1010.07	2.67126E+07	401.837
34.2996	.342996	.109	1066.85	212041	407.83
35.2344	.352344	.208	1139.02	54751.8	415.019
36.4317	.364317	.307	1234.5	23479.1	423.796
37.7555	.377555	.406	1367.97	12439.1	434.764
39.3337	.393337	.505	1570.37	7370.28	448.917
41.2786	.412786	.604	1920.57	4653.78	468.049
43.7981	.437981	.703	2700.79	3035.76	495.843
47.3477	.473477	.802	6315.3	1987.04	541.671
53.317	.53317	.901	3.35E+08	1248.37	598.897
98.087	.98087	1	3.35E+08	344.897	727.705

% B REACTED= 98.087 TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>_

Table 5-22

Estimated Cure Path Properties of 2 Moles of TGMDA and 1 Mole of DDS (see Table 5-7)

```
A AND B COREACTION-MOL. WT. DIST.-THERMAL TRANS -D.H KAELBLE-OCT
. 27,1982
IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS
MOLES OF TYPE A (MOLE)=? 1
TYPE A FUNTIONALITY(=>2)=? 4
MOL WT. OF TYPE A (G/MOLE)=? 248
MOLES OF TYPE B (MOLE)=? 2
TYPE B FUNCTIONALITY (=>2)=? 4
MOL WT. OF TYPE B (G/MOLE)=? 422
FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 1
NUMBER OF A AND B MAIN CHAIN ATOMS (A1,A2)=? 11,17
MOL WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 5168
GLASS COORDINATION NUMBER (3<Z<10)=? 10
MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T1,T2) IN DEG K=
? 260,583
GEL POINT (% A REACTED)= 66.6657
GEL POINT (% B REACTED)= 33.3333
INITIAL NUM. AVE. DEG OF POLYMERIZATION= 2.6749
TO ANALYSE POLYMERIZATION PRESS ENTER?
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% A REACTED	BRANCH COEF.	NUM AVE MW(G/MOL)	WT. AVE MW(G/MOL)	GLASS TEMP(K)	FLOW TEMP(K)
0	0	364	364	260	263.065
6.65334	.0332667	389.944	417.806	268.535	277.179
13.3067	.0665334	419.871	485.93	277.962	286.934
19.96	.0998009	454.773	571.497	287.747	297.407
26.6134	.133067	496.003	686.479	298.36	308.694
33.2667	.166333	545.455	847.397	309.736	320.913
39.92	.1996	605.859	1088.37	322.123	334.215
46.5734	.232867	681.308	1488.93	335.482	348.829
53.2267	.266134	778.222	2286.08	349.939	365.143
59.8801	.2994	907.279	4645.22	365.327	384.175
66.5334	.332667	1092.63	242657	393.135	475.197

```
TO ANALYSE CROSSLINKING PRESS ENTER?
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%A REACTED	BRANCH COEF.	WT. FR. GEL	NUM. AVE. MW(G/MOL)	X-LINK MW (G/MOL)	GLASS TEMP(K)
66.8339	.334169	-.0100001	1097.51	2.90251E+07	383.978
68.5993	.342996	.109	1159.21	230396	388.993
70.5888	.352944	.208	1237.62	59491.5	395.02
72.8634	.364317	.307	1341.36	25511.6	402.332
75.5111	.377555	.406	1486.39	13515.9	411.572
78.6674	.393337	.505	1706.31	8008.31	423.393
82.5573	.412786	.604	2086.63	5056.65	439.291
87.5962	.437981	.703	2934.59	3298.56	462.172
94.6954	.473477	.802	6861.99	2159.05	499.291
99.9268	.499632	.85348	435168	1709.73	530.892

```
% B REACTED= 49.9632 .TO CONTINUE TYPE RUN AND PRESS ENTER
READY
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Table 5-23 SC5291.7FR

Estimated Cure Path for TGMDA Homopolymer
(see Table 5-8)

A AND B COREACTION-MOL. WT. DIST -THERMAL TRANS -D.H.KAELBLE-OCT 27,1982
IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS
MOLES OF TYPE A (MOLE)=? 1
TYPE A FUNTIONALITY(=>2)=? 4
MOL. WT. OF TYPE A (G/MOLE)=? 422
MOLES OF TYPE B (MOLE)=? 1
TYPE B FUNCTIONALITY (=>2)=? 4
MOL. WT. OF TYPE B (G/MOLE)=? 422
FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 1
NUMBER OF A AND B MAIN CHAIN ATOMS (A1,A2)=? 17,17
MOL. WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 5300
GLASS COORDINATION NUMBER (8<Z<10)=? 10
MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T1,T2) IN DEG. K=? 260,402
GEL POINT (% A REACTED)= 33.3333
GEL POINT (% B REACTED)= 33.3333
INITIAL NUM. AVE. DEG. OF POLYMERIZATION= 4.55742
TO ANALYSE POLYMERIZATION PRESS ENTER?

% A REACTED	BRANCH COEF.	NUM. AVE. MW(G/MOL)	WT. AVE. MW(G/MOL)	GLASS TEMP(K)	FLOW TEMP(K)
0	0	422	422	260	268.5
3.32667	.0332667	452.878	484.38	266.258	275.243
6.65334	.0665334	486.773	562.315	272.824	282.344
9.98001	.0998001	527.237	662.455	279.722	289.84
13.3067	.133067	575.037	795.863	286.978	297.73
16.6333	.166333	632.368	982.422	294.621	306.226
19.96	.1996	702.397	1261.79	302.681	315.259
23.2867	.232867	789.888	1726.18	311.196	325.057
26.6134	.266134	902.224	2550.35	320.203	335.892
29.94	.2994	1051.85	5306.56	329.747	348.693
33.2667	.332667	1260.96	281322	339.877	437.952

TO ANALYSE CROSSLINKING PRESS ENTER? _

%A REACTED	BRANCH COEF.	WT. FR. GEL	NUM. AVE. MW(G/MOL)	X-LINK MW (G/MOL)	GLASS TEMP(K)
33.4169	.334169	.0100001	1272.38	3.365E+07	340.351
34.2996	.342996	.109	1343.92	267108	343.267
35.2944	.352944	.208	1434.83	68970.9	346.821
36.4317	.364317	.307	1555.1	29576.7	351.202
37.7555	.377555	.406	1723.23	15669.5	356.595
39.3337	.393337	.505	1978.19	9284.36	363.753
41.2786	.412786	.604	2419.35	5862.38	373.166
43.7981	.437981	.703	3402.19	3824.16	386.481
47.3477	.473477	.802	7955.39	2583.07	407.368
53.317	.53317	.901	4.22E+08	1562.5	431.108
98.087	.98087	1	4.22E+08	434.467	530.321

% B REACTED= 98.087 TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>_

Table 5-24

Estimated Polymerization Path for Equimolar Isoamyl-Neopentyl Acrylate Copolymer (see Table 5-9)

```
A AND B COREACTION-MOL. WT. DIST -THERMAL TRANS.-D H.KAELBLE-OCT
. 27,1982
IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS
MOLES OF TYPE A (MOLE)=? 1
TYPE A FUNTIONALITY(=>2)=? 2
MOL. WT. OF TYPE A (G/MOLE)=? 142
MOLES OF TYPE B (MOLE)=? 1
TYPE B FUNCTIONALITY (=>2)=? 2
MOL. WT. OF TYPE B (G/MOLE)=? 142
FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 0
NUMBER OF A AND B MAIN CHAIN ATOMS (A1,A2)=? 2,2
MOL. WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 34185
GLASS COORDINATION NUMBER (0<Z<10)=? 10
MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T1,T2) IN DEG. K=
? 69,240
GEL POINT (% A REACTED)= 100
GEL POINT (% B REACTED)= 100
INITIAL NUM. AVE. DEG. OF POLYMERIZATION= 1.03377
TO ANALYSE POLYMERIZATION PRESS ENTER? _
```

% A REACTED	BRANCH COEF.	NUM. AVE MW(G/MOL)	WT. AVE MW(G/MOL)	GLASS TEMP.(K)	FLOW TEMP(K)
0	0	142	142	69	70.8494
9.98001	9.96006E-03	143.429	144.857	69.4932	71.3977
19.96	.0399402	147.892	153.784	71.0159	73.0965
29.94	.0896405	155.982	169.955	73.7076	76.0586
39.92	.159361	168.919	195.838	77.9381	80.591
49.9	.249001	189.002	236.163	83.8818	87.1751
59.8801	.358562	221.379	300.755	92.6766	96.5839
69.8601	.488043	277.367	412.734	105.785	110.755
79.8401	.637444	391.663	641.327	126.415	132.784
89.8201	.806765	734.855	1327.71	162.284	171.119
99.8001	.996006	35552.9	70963.8	237.548	264.313

```
% B REACTED= 99.8001   TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>_
```

Table 5-25

Estimated Polymerization Path for Polystyrene

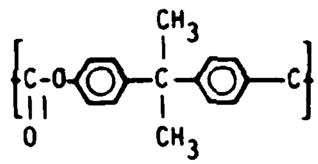
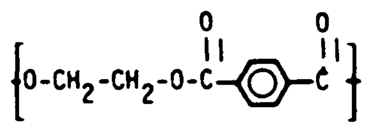
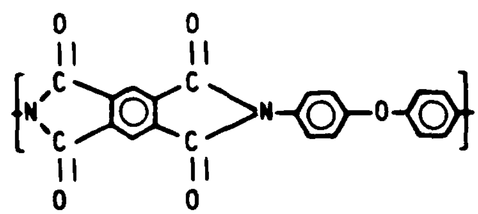
```
A AND B COREACTION-MOL. WT. DIST.-THERMAL TRANS.-D H KAELBLE-OCT
 27,1982
IF NONSTOICHIOMETRIC REACTION HAVE MOLES OF B IN EXCESS
MOLES OF TYPE A (MOLE)=? 1
TYPE A FUNTIONALITY(=>2)=? 2
MOL. WT. OF TYPE A (G/MOLE)=? 104
MOLES OF TYPE B (MOLE)=? 1
TYPE B FUNCTIONALITY (=>2)=? 2
MOL. WT. OF TYPE B (G/MOLE)=? 104
FRACTION OF MOLECULES OF FUNCTIONALITY >2=? 0
NUMBER OF A AND B MAIN CHAIN ATOMS (A1,A2)=? 2,2
MOL. WT. BETWEEN ENTANGLEMENTS (G/MOLE)=? 20200
GLASS COORDINATION NUMBER (8<Z<10)=? 10
MONOMER AND LINEAR POLYMER GLASS TEMPERATURES (T1,T2) IN DEG. K=
? 110,384
GEL POINT (% A REACTED)= 100
GEL POINT (% B REACTED)= 100
INITIAL NUM. AVE. DEG. OF POLYMERIZATION= 1.00365
TO ANALYSE POLYMERIZATION PRESS ENTER? _
```

% A REACTED	BRANCH COEF.	NUM. AVE MW(G/MOL)	WT. AVE MW(G/MOL)	GLASS TEMP(K)	FLOW TEMP(K)
0	0	104	104	110	111.849
9.98001	9.96006E-03	105.046	106.093	110.787	112.692
19.96	.0398402	108.315	112.631	113.219	115.239
29.94	.0896405	114.241	124.481	117.517	119.863
39.92	.159361	123.715	143.431	124.113	126.866
49.9	.243001	138.492	172.965	133.767	137.06
59.8801	.359562	162.136	220.271	147.919	151.827
69.8601	.488043	203.142	302.284	158.774	173.744
79.8401	.637444	286.052	469.784	201.777	208.145
89.8201	.806765	538.204	972.408	259.226	268.061
99.8001	.996006	26030.7	51973.5	380.217	407.779

```
% B REACTED= 99.8001   TO CONTINUE TYPE RUN AND PRESS ENTER
READY
>_
```

Table 6-1

Chemical Structure and Thermal Transitions of Six Film Forming Polymers

No.	Repeat Unit Structure	Thermal Transition (K) T_γ	T_g	T_c
1	$\left[CF_2 - CF_2\right]_x \left[CF_2 - \underset{\displaystyle CF}{\overset{\displaystyle CF_3}{\vert}}\right]_{0.14x}$	177	358	555
2	$-CF_2-CF_2-$	177	400	600
3	$\left[CF_s - \underset{\displaystyle CF}{\overset{\displaystyle Cl}{\vert}}\right]_x \left[CF_2 - CH_2\right]_{0.03x}$	273	323	493
4		176	423	538
5		243	350	536
6		180	530	-

T_λ is an amorphous transition below T_g involving local motion of 2-4 atoms.
T_g is the amorphous glass transition involving cooperative motion of 20-40 atoms in chain segments.
T_c is the crystalline phase melting temperature involving cooperative motion of the entire polymer molecule.

Table 6-2
Input Format for Chemical-Mechanical Property Program
(Upper symbols found in Ref. 1 and lower symbols in Table 6-3)

		C1	C2	C3	C4	C5
	R1	Polymer or Experiment Name AO$				
Polymer Properties	R2	M_p (g/mol) AA	X_p (mole) AB	Σh_p AC	ρ_p (g/cc) AD	$(T_{gAR})_P$ (K) AE
	R3	Z_{gP} AF	V^o_{gP} (cc/mol) AG	q_{LP} AH	δ_P $(cal/cc)^{1/2}$ AI	AR_P (S^{-1}) AJ
	R4	M_o (g/mol) AK	M_c (g/mol) AL	M_e (g/mol) AM	τ_g (S) AN	ϕ AP
Diluent Properties	R5	M_D (g/mol) AQ	X_D (mol) AR	Σh_D AS	ρ_D (g/cc) AT	$(T_{gAR})_D$ (K) AU
	R6	Z_{gD} AV	V^o_{GD} (cc/mol) AW	q_{LD} AX	δ_D $(cal/cc)^{1/2}$ AY	AR_D (S^{-1}) AZ
Use Condition	R7	A (S^{-1}) BA	t_I (S) BB	T (K) BC	ΔT (K) BD	NT BE

Table 6-3

Input Nomenclature for Chemical-Mechanical Program

Row	Symbol	Meaning
2	AA	Polymer molecular weight (number ave.)
	AB	Moles polymer
	AC	Polymer repeat unit rotational degrees of freedom
	AD	Polymer density
	AE	Polymer glass temperature at reference strain rate AJ
3	AF	Total adjacent lattice (Z) sites for glass (nominally = 10)
	AG	Polymer glass repeat unit molar volume
	AH	Intermolecular lattice sites in polymer liquid (nominally = 9)
	AI	Polymer solubility parameter
	AJ	Strain (or thermal scan) rate for reference polymer glass temperature (nominally = 1.0)
4	AK	Polymer repeat unit molecular weight
	AL	Molecular weight between crosslinks (number ave.)
	AM	Molecular weight between entanglements (number ave.)
	AN	Relaxation time at T_g (nominally = 1.0)
	AP	Polymer-diluent interaction parameters (nominally = 1.0)
5	AQ	Diluent molecular weight
	AR	Moles diluent
	AS	Diluent molecular rotational degrees of freedom
	AT	Diluent density
	AU	Diluent glass temperature at reference rate AZ
6	AV	Total adjacent lattice (Z) sites of diluent glass (nominally = 10)
	AW	Diluent glass molar volume
	AX	Intermolecular lattice (q) sites of diluent liquid (nominally = 9)
	AY	Diluent solubility parameter
	AZ	Strain (or thermal scan) rate for diluent reference glass temperature (nominally = 1.0)
7	BA	Mechanical (or thermal scan) strain rate (nominally = 1.0)
	BB	Constant time for isochronal stress-strain response (nominally = 1.0)
	BC	Starting temperature for family of stress-strain curves
	BD	Temperature increment
	BE	Number of temperatures

Table 6-4
Nomenclature for Intermediate Results in
Chemical-Mechanical Program

Line No.	Symbol	Meaning
1	BF	Wood constant in T_g calculation
	BG	Rate ratio in polymer T_g calculation
	BH	Log BG
	BI	Polymer T_g at rate BA (K)
	BJ	Polymer T_g change with shear stress (K/bar)
2	BK	Rate ratio in diluent T_g calculation
	BL	Log BK
	BM	Diluent T_g at rate BA (K)
	BN	Diluent T_g change with shear stress (K/bar)
3	TG	T_g of polymer-diluent at zero stress (K)
	UR	Polymer-diluent T_g change with shear stress (K/bar)
4	BO	Volume fraction polymer
	BQ	Volume fraction diluent
	BR	Cohesive energy of polymer-diluent solution (cal/cc)
5	BS	Fraction of effective crosslinked segments
	BT	Fraction of effective entangled segments
6	BU	Glass state shear modulus (bar)
	BV	Rubber state shear modulus at τ_g (bar)
	BX	Rubber state shear modulus at τ_l (bar)
	BY	Rubber state shear modulus at τ_m (bar)
	BZ	Crosslink network shear modulus (bar)
7	SB	Brittle shear strength (bar)
	TL	$\log_{10} (\tau_m/\tau_g)$
	TM	Melt (or flow) temperature (K)
	NH	Fraction Neohookian versus Hookian tensile response
8	T	Current temperature (K)
	SM	Flow shear strength (bar)
	SS	Current shear strength (bar)

Table 6-5
Estimated Mechanical Properties of an Acrylate Copolymer

```
POLYMER-DILUENT=EQUIMOLAR ISOAMYL-NEOPENTYL ACRYLATE
POLYMER PROPERTIES:
AA,AB,AC,AD,AE= 1.03E+06  1  121  1.09  230
AF,AG,AH,AI,AJ= 10  260  9  9.07  1
AK,AL,AM,AN,AP= 284  1.03E+06  34200  1  1
DILUENT PROPERTIES
AQ,AR,AS,AT,AU= 284  0  121  1.09  59
AV,AW,AX,AY,AZ= 10  260  9  9.07  1
TEST CONDITIONS:
BA,BB,BC,BD,BE= 1  1  100  25  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 1  1  0  230  .114881
BK,BL,BM,BN= 1  0  59  .114881
TG,UR= 230  .114881
BO,BQ,BR= 1  0  82.2649
BS,BT= 0  .933592
BU,BV,BX,BY,BZ= 27547.9  27547.9  .609377  .157335  0
SB,TL,TM,NH= 960.491  12.1372  349.002  0
T,SM,BS= 100  2157.48  860.491
SHEAR AND TENSION ANALYSIS.
INPUT NUMBER OF STRESS INCREMENTS? 12_

INPUT NUMBER OF STRESS INCREMENTS? 12
```

SHEAR MODULUS (BAR)	SHEAR STRESS (BAR)	SHEAR STRAIN	TENSILE STRESS (BAR)	TENSILE STRAIN
	0	0	0	0
27547.9	71.7076	2.60301E-03	143.415	1.73534E-03
27547.9	143.415	5.20603E-03	286.83	3.47069E-03
27547.9	215.123	7.80904E-03	430.245	5.20603E-03
27547.9	286.83	.0104121	573.661	6.94137E-03
27547.9	358.538	.0130151	717.076	8.67672E-03
27547.9	430.245	.0156181	860.491	.0104121
27547.9	501.953	.0182211	1003.91	.0121474
27547.9	573.661	.0208241	1147.32	.0138827
27547.9	645.368	.0234271	1290.74	.0156181
27547.9	717.076	.0260301	1434.15	.0173534
27547.9	788.783	.0286332	1577.57	.0190888
27547.9	860.491	.0312362		

```
SHEAR FAILURE PROPERTIES:
STRESS(BAR)= 860.491 STRAIN= .0312362   ENERGY/VOL(BAR)=
 11.2927
E-MODULUS(BAR)= 27147.9        E-WORK(BAR)= 11.2927
E-STRAIN= .0312362             P-WORK(BAR)= 0

TENSILE FAILURE PROPERTIES:
STRESS(BAR)= 1636.56 STRAIN= .0204074   ENERGY/VOL(BAR)=
 17.2091
E-MODULUS(BAR)= 82543.7        E-WORK(BAR)= 17.2091
E-STRAIN= .0204074             P-WORK(BAR)= 0
PRESS ENTER TO CONTINUE ? _
```

Table 6-6
Calculated Effects of Isochronal Loading Time t Upon the Shear and Tensile Failure Properties of Equimolar Isoamyl-Neopentyl Acrylate Linear Polymer (M_n = 1.06 E6) at T = 296K with Hookian Response

	Shear			Tension		
t (S)	σ_b (bar)	γ_b	W_S (bar)	S_b (bar)	ϵ_b	W_T (bar)
2E2	9.6	55	243	2.82	5.8	8.19
1E2	52.4	334	8.3E3	7.37	13.2	48.7
1E1	224	1200	1.35E5	19.3	22.2	215
1	461	2156	5.2E5	34.5	25.8	444
1E-2	860	2310	1.13E6	107	15.1	806
1E-4	860	582	3.08E5	278	5.2	814
1E-5	860	186	9.88E4	441	3.2	791
1E-6	860	58	3.1E4	582	1.96	726
1E-8	860	5.9	3.1E3	1010	0.70	491
1E-10	860	0.58	312	1449	0.18	196
1E-12	860	0.067	32	1664	0.033	35.9
1E-14	860	0.034	13.5	1686	0.020	17.2

Table 6-7
Estimated Effects of Low Moisture (0 - 2 Wt%) on Cured Epoxy Thermoset

```
POLYMER-DILUENT=TGMDA/DDS EPOXY+0% H2O
POLYMER PROPERTIES:
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES:
AQ,AR,AS,AT,AU= 18  0  20  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS:
BA,BB,BC,BD,BE= 1  1  300  25  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 3.81052  1  0  483  .158045
BK,BL,BM,BN= 1  0  137  .0393688
TG,UR= 483  .158045
BO,BQ,BR= 1  0  158.76
BS,BT= .993095  .979119
BU,BV,BX,BY,BZ= 53163.7  53163.7  9.8124  1.30231  35.8285
SB,TL,TM,NH= 1660.63  11.5743  585.517  0
T,SM,SS= 300  1806.56  1660.63
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _

POLYMER-DILUENT=TGMDA/DDS EPOXY+2% H2O
POLYMER PROPERTIES:
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES:
AQ,AR,AS,AT,AU= 18  550  20  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS:
BA,BB,BC,BD,BE= 1  1  300  25  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 3.81052  1  0  483  .158045
BK,BL,BM,BN= 1  0  137  .0393688
TG,UR= 458.498  .149641
BO,BQ,BR= .977326  .022674  156.065
BS,BT= .993095  .978635
BU,BV,BX,BY,BZ= 52261.1  51958.2  8.36124  1.22215  33.2358
SB,TL,TM,NH= 1632.44  11.5956  561.582  0
T,SM,SS= 300  1748.06  1632.44
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _
```

Table 6-8

Estimated Effects of Medium Moisture (4 - 6 Wt%) on Cured Epoxy Thermoset

```
POLYMER-DILUENT=TGMDA/DDS EPOXY+4% H2O
POLYMER PROPERTIES
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES
AQ,AR,AS,AT,AU= 18  1100  20  1  137
AV,AW,AX,AY,AZ= 10  13  11  23.2  1
TEST CONDITIONS:
BA,BB,BC,BD,BE= 1  1  300  25  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE


INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 3.81052  1  0  483  .158045
BK,BL,BM,BN= 1  0  137  .0393688
TG,UR= 437.238  .142349
BO,BQ,BR= .955658  .0443425    153.979
BS,BT= .993095  .97815
BU,BV,BX,BY,BZ= 51562.6  50806.3  7.29674  1.15249  30.9882
SB,TL,TM,NH= 1610.62  11.6135  548.799  0
T,SM,SS= 300  1691.61  1610.62
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _


POLYMER-DILUENT=TGMDA/DDS EPOXY+6% H2O
POLYMER PROPERTIES:
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES:
AQ,AR,AS,AT,AU= 18  1650  20  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS:
BA,BB,BC,BD,BE= 1  1  300  25  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE


INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 3.81052  1  0  483  .158045
BK,BL,BM,BN= 1  0  137  .0393688
TG,UR= 418.614  .135961
BO,BQ,BR= .934929  .0650711    152.432
BS,BT= .993095  .977666
BU,BV,BX,BY,BZ= 51044.5  49704.3  7.30274  1.09137  29.0213
SB,TL,TM,NH= 1594.43  11.6284  522.577  0
T,SM,SS= 300  1637.07  1594.43
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _
```

Table 6-9

Estimated Effects of High Moisture (8 - 10 Wt%) on Cured Epoxy Thermoset

```
POLYMER-DILUENT=TMDA/DDS EPOXY+8% H2O
POLYMER PROPERTIES
AA,AB,AC,AD,AE= 495000  1 .319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.5  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES
AQ,AR,AS,AT,AU= 18  2200  20  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS
BA,BB,BC,BD,BE= 1  1  300  25  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE


INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 3.81052  1  0  483  .158045
BK,BL,BM,BN= 1  0  137  .0393688
TG,UR= 402.166  .130319
BO,BQ,BR= .915001  .0849195        151.361
BS,BT= .993095  .977122
BU,BV,BX,BY,BZ= 50685.9  48649  6.86686  1.0373  27.2858
SB,TL,TM,NH= 1583.23  11.6409  506.465  0
T,SM,SS= 300  1594.3  1583.23
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _


POLYMER-DILUENT=TGMDA/DDS EPOXY+10% H2O
POLYMER PROPERTIES:
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES
AQ,AR,AS,AT,AU= 18  2750  20  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS:
BA,BB,BC,BD,BE= 1  1  300  25  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE


INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 3.81052  1  0  483  .158045
BK,BL,BM,BN= 1  0  137  .0393688
TG,UR= 387.534  .125301
BO,BQ,BR= .896057  .103943        150.711
BS,BT= .993095  .976697
BU,BV,BX,BY,BZ= 50468.4  47637.7  6.47946  .989109  25.7433
SB,TL,TM,NH= 1576.44  11.6512  492.112  0
T,SM,SS= 300  1533.21  1533.21
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _
```

Table 6-10

Second Estimated Effects of Low Moisture (0 - 2 Wt%) on Cured Epoxy Thermoset

```
POLYMER-DILUENT=TGMDA/DDS EPOXY+0% H2O
POLYMER PROPERTIES
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES:
AQ,AR,AS,AT,AU= 18  0  28  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS
BA,BB,BC,BD,BE= 1  1  220  40  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 5.33473  1  0  483  158045
BK,BL,BM,BN= 1  0  137  .0281206
TG,UR= 483  158045
BO,BQ,BR= 1  0  158.76
BS,BT= .993095  .979119
BU,BV,BX,BY,BZ= 53163.7  53163.7  9.0124  1.30231  35.8285
SB,TL,TM,NH= 1660.63  11.5743  585.517  0
T,SM,SS= 220  2312.74  1660.63
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _

POLYMER-DILUENT=TGMDA/DDS EPOXY+2% H2O
POLYMER PROPERTIES:
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES:
AQ,AR,AS,AT,AU= 18  550  28  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS:
BA,SB,BC,BD,BE= 1  1  220  40  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE

INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 5.33473  1  0  483  .158045
BK,BL,BM,BN= 1  0  137  .0281206
TG,UR= 449.643  .145519
BO,BQ,BR= .977326  .022674  156.065
BS,BT= .993095  .978635
BU,BV,BX,BY,BZ= 52261.1  51959.2  8.19975  1.19854  32.5939
SB,TL,TM,NH= 1632.44  11.6126  553.179  0
T,SM,SS= 220  2289.59  1632.44
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _
```

Table 6-11

Second Estimated Effects of Medium Moisture (4 - 6 Wt%) on Cured Epoxy Thermoset

```
POLYMER-DILUENT=TGMDA/DDS EPOXY+4% H2O
POLYMER PROPERTIES:
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES:
AQ,AR,AS,AT,AU= 18  1100  28  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS:
BA,BB,BC,BD,BE= 1  1  220  40  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE


INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 5.33473  1  0  483   .158045
BK,BL,BM,BN= 1  0  137  .0281206
TG,UR= 422.152  .135196
BO,BQ,BR= .955658  .0443425      153.979
BS,BT= .993095  .97815
BU,BV,BX,BY,BZ= 51562.6  50806.3  7.52773  1.11272  29.919
SB,TL,TM,NH= 1610.62  11.644  526.535  0
T,SM,SS= 220  2267.33  1610.62
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _


POLYMER-DILUENT=TGMDA/DDS EPOXY+6% H2O
POLYMER PROPERTIES:
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES:
AQ,AR,AS,AT,AU= 18  1650  28  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS:
BA,BB,BC,BD,BE= 1  1  220  40  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE


INTERMEDIATE RESULTS:
BF,BG,BH,BI,BJ= 5.33473  1  0  483  .158045
BK,BL,BM,BN= 1  0  137  .0281206
TG,UR= 399.105  .126542
BO,BQ,BR= .934929  .0650711      152.432
BS,BT= .993095  .977666
BU,BV,BX,BY,BZ= 51044.5  49704.3  6.9624  1.0405  27.6687
SB,TL,TM,NH= 1594.43  11.6699  504.193  0
T,SM,SS= 220  2245.84  1594.43
SHEAR AND TENSION ANALYSIS:
INPUT NUMBER OF STRESS INCREMENTS? _
```

Table 6-12

Second Estimated Effects of High Moisture (8 - 10 Wt%) on Cured Epoxy Thermoset

```
POLYMER-DILUENT=TGMDA/DDS EPOXY+8% H2O
POLYMER PROPERTIES
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES
AQ,AR,AS,AT,AU= 18  2200  28  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS
BA,BB,BC,BD,BE= 1  1  220  40  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0


INTERMEDIATE RESULTS
BF,BG,BH,BI,BJ= 5.33473  1  0  483  .158045
BK,BL,BM,BN= 1  0  137  .0281206
TG,UR= 379.504  .119182
BO,BQ,BR= .915081  .0849195      151.361
BS,BT= .993095  .977162
BU,BV,BX,BY,BZ= 50685.9  48649  6.47992  .978844  25.7482
SB,TL,TM,NH= 1583.23  11.6913  485.179  0
T,SM,SS= 220  2225  1583.23
SHEAR AND TENSION ANALYSIS
INPUT NUMBER OF STRESS INCREMENTS? _


POLYMER-DILUENT=TGMDA/DDS EPOXY+10% H2O
POLYMER PROPERTIES
AA,AB,AC,AD,AE= 495000  1  319  1.16  483
AF,AG,AH,AI,AJ= 10  943  9  12.6  1
AK,AL,AM,AN,AP= 1094  1709  5168  1  .32
DILUENT PROPERTIES
AQ,AR,AS,AT,AU= 18  2750  28  1  137
AV,AW,AX,AY,AZ= 10  18  11  23.2  1
TEST CONDITIONS
BA,BB,BC,BD,BE= 1  1  220  40  15
FRACTION NEOHOOKIAN TENSILE RESPONSE= 0
PRESS ENTER TO CONTINUE


INTERMEDIATE RESULTS
BF,BG,BH,BI,BJ= 5.33473  1  0  483  158045
BK,BL,BM,BN= 1  0  137  .0281206
TG,UR= 362.632  .112846
BO,BQ,BR= .896057  .103943      150.711
BS,BT= .993095  .976697
BU,BV,BX,BY,BZ= 50468.4  47637.7  6.0631  .925551  24.0891
SB,TL,TM,NH= 1576.44  11.7089  468.793  0
T,SM,SS= 220  2204.71  1576.44
SHEAR AND TENSION ANALYSIS
INPUT NUMBER OF STREGS INCREMENTS? _
```

Table 6-13

Calculated Mechanical Response of Cured TGMDA/DDS Epoxy (0 Wt% H_2O, T_g = 483K, t = 1 s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.66E3	2.24E-2	1.85E1	1.85E1	0	7.39E4	2.34E-2
260	1.66E3	2.24E-2	1.85E1	1.85E1	0	7.39E4	2.34E-2
300	1.66E3	3.22E-2	3.42E1	1.92E1	1.50E1	7.17E4	2.32E-2
340	1.55E3	1.31E-1	1.77E2	2.81E1	1.49E2	4.30E4	3.61E-2
380	1.30E3	2.30E-1	2.56E2	4.29E1	2.13E2	1.97E4	6.59E-2
420	1.05E3	3.61E-1	3.02E2	7.55E1	2.26E2	7.27E3	1.44E-1
460	7.94E2	5.94E-1	3.25E2	1.46E2	1.78E2	2.15E3	3.70E-1
500	5.41E2	9.27E-1	2.01E2	2.01E2	0	4.67E2	9.27E-1
540	2.88E2	1.08	7.80E1	7.80E1	0	1.35E2	1.08
580	3.49E1	4.84E-1	7.46	7.46	0	6.36E1	4.84E-1
585	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.27E3	1.47E-2	2.40E1	2.40E1	0	2.22E5	1.47E-2
260	3.27E3	1.47E-2	2.40E1	2.40E1	0	2.22E5	1.47E-2
300	3.26E3	1.94E-2	3.89E1	2.44E1	1.45E1	2.18E5	1.49E-2
340	2.94E3	5.64E-2	1.40E2	2.56E1	1.14E2	1.69E5	1.74E-2
380	2.37E3	9.66E-2	2.01E2	2.80E1	1.73E2	1.00E5	2.36E-2
420	1.80E3	1.61E-1	2.48E2	4.24E1	2.05E2	3.85E4	4.70E-2
460	1.25E3	2.71E-1	2.55E2	8.29E1	1.73E2	9.42E3	1.33E-1
500	7.20E2	5.03E-1	1.64E2	1.64E2	0	1.30E3	5.03E-1
540	3.53E2	6.30E-1	6.39E1	6.39E1	0	3.22E2	6.30E-1
580	5.49E1	2.72E-1	6.76	6.76	0	1.83E2	2.71E-1
585	0	0	0	0	0	0	0

Table 6-14
Calculated Mechanical Response of 2 Wt% Moisture
in Cured Epoxy (T_g = 449.6K, t = 1 s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.63E3	2.23E-2	1.82E1	1.82E1	0	7.26E4	2.24E-2
260	1.63E3	2.23E-2	1.82E1	1.82E1	0	7.26E4	2.24E-2
300	1.63E3	8.79E-2	1.21E2	2.26E1	9.03E1	5.89E4	2.77E-2
340	1.46E3	1.85E-1	2.29E2	4.24E1	1.87E1	2.53E4	5.79E-2
380	1.19E3	3.43E-1	3.30E2	7.76E1	2.53E2	9.12E3	1.30E-1
420	9.15E2	3.36E-1	1.90E2	1.18E2	7.18E1	3.56E3	2.57E-1
460	6.40E2	8.26E-1	2.25E2	2.25E2	0	6.61E2	8.26E-1
500	3.65E2	1.18	9.28E1	9.28E1	0	1.34E2	1.18
540	9.05E1	8.49E-1	2.76E1	2.76E1	0	7.66E1	8.49E-1
553	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.22E3	1.47E-2	2.36E1	2.36E1	0	2.18E5	1.47E-2
260	3.22E3	1.47E-2	2.36E1	2.36E1	0	2.18E5	1.47E-2
300	3.15E3	3.69E-2	9.16E1	2.46E1	6.70E1	2.02E5	1.56E-2
340	2.71E3	8.29E-2	1.91E2	3.36E1	1.58E2	1.10E5	2.47E-2
380	2.08E3	1.45E-1	2.54E2	4.71E1	2.08E2	4.59E4	4.53E-2
420	1.53E3	1.95E-1	2.04E2	9.44E1	1.10E2	1.24E4	1.23E-1
460	8.72E2	4.69E-1	2.12E2	1.96E2	1.61E1	1.94E3	4.50E-1
500	4.27E2	7.13E-1	8.40E1	8.40E1	0	3.30E2	7.13E-1
540	1.23E2	4.74E-1	2.30E1	2.30E1	0	2.05E2	4.74E-1
553	0	0	0	0	0	0	0

Table 6-15
Calculated Mechanical Response of 4 Wt% Moisture in Cured Epoxy (T_g = 422K, t = 1 s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.61E3	2.24E-2	1.80E1	1.80E1	0	7.17E4	2.24E-2
260	1.61E3	2.24E-2	1.80E1	1.80E1	0	7.17E4	2.24E-2
300	1.61E3	1.72E-1	2.36E2	4.08E1	1.95E2	3.18E4	5.06E-2
340	1.38E3	3.20E-1	3.65E2	7.75E1	2.87E2	1.23E4	1.12E-1
380	1.08E3	5.21E-1	4.24E2	1.40E2	2.84E2	4.19E3	2.59E-1
420	7.88E2	7.41E-1	3.06E2	2.78E2	2.75E1	1.12E3	7.06E-1
460	4.92E2	1.15	1.04E2	1.04E2	0	1.58E2	1.15
500	1.96E2	1.09	5.75E1	5.75E1	0	9.72E1	1.09
527	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.17E3	1.47E-2	2.33E1	2.33E1	0	2.15E5	1.47E-2
260	3.17E3	1.47E-2	2.33E1	2.33E1	0	2.15E5	1.47E-2
300	2.99E3	7.61E-2	1.95E2	3.26E1	1.63E2	1.37E5	2.18E-2
340	2.43E3	1.35E-1	2.84E2	4.43E1	2.40E2	6.67E4	3.65E-2
380	1.78E3	2.20E-1	3.14E2	7.61E1	2.38E2	2.07E4	8.57E-2
420	1.13E3	3.96E-1	2.85E2	1.62E2	1.23E2	3.94E3	2.87E-1
460	5.77E2	7.04E-1	9.07E1	9.07E1	0	3.66E2	7.04E-1
500	2.39E2	6.39E-1	4.99E1	4.99E1	0	2.44E2	6.39E-1
527	0	0	0	0	0	0	0

Table 6-16
Calculated Mechanical Response of 6 Wt% Moisture in Cured Epoxy (T_g = 399K, t = 1 s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.59E3	2.24E-2	1.78E1	1.78E1	0	7.09E4	2.24E-2
260	1.59E3	3.32E-2	3.28E1	1.85E1	1.44E1	6.88E4	2.32E-2
300	1.59E3	1.15E-1	1.34E2	4.85E1	8.57E1	2.62E4	6.08E-2
340	1.30E3	4.35E-1	4.45E2	1.20E2	3.25E2	7.04E3	1.84E-1
380	9.81E2	6.71E-1	4.33E2	2.26E2	2.06E2	2.13E3	4.61E-1
420	6.65E2	1.02	2.11E2	2.11E2	0	4.04E2	1.02
460	3.49E2	1.13	6.77E1	6.77E1	0	1.07E2	1.13
500	3.31E1	5.56E-1	7.89	7.89	0	5.11E1	5.56E-1
504	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.14E3	1.47E-2	2.30E1	2.30E1	0	2.13E5	1.47E-2
260	3.13E3	1.94E-2	3.74E1	2.34E1	1.40E1	2.09E5	1.50E-2
300	2.98E3	7.17E-2	1.65E2	4.89E1	1.15E2	9.06E4	3.28E-2
340	2.20E3	1.81E-1	3.31E2	6.60E1	2.64E2	3.66E4	6.01E-2
380	1.50E3	3.06E-1	3.32E2	1.28E2	2.03E2	8.80E3	1.71E-1
420	8.29E2	6.05E-1	2.05E2	2.06E2	0	1.12E3	6.05E-1
460	4.03E2	7.35E-1	8.15E1	8.15E1	0	3.02E2	7.35E-1
500	5.06E1	3.09E-1	6.96	6.96	0	1.46E2	3.09E-1
504	0	0	0	0	0	0	0

Table 6-17
Calculated Mechanical Response of 8 Wt% Moisture in Cured Epoxy (T_g = 380K, t = 1 s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.58E3	2.24E-2	1.77E1	1.77E1	0	7.04E4	2.24E-2
260	1.58E3	7.64E-2	9.99E1	2.11E1	7.88E1	5.94E4	2.66E-2
300	1.55E3	3.49E-1	4.42E2	1.01E2	3.41E2	1.20E4	1.30E-1
340	1.22E3	3.79E-1	3.21E2	1.40E2	1.81E2	5.32E3	2.29E-1
380	8.82E2	4.59E-1	1.56E2	1.56E2	0	1.48E3	4.59E-1
420	5.47E2	1.19	8.62E1	8.62E1	0	1.22E2	1.19
460	2.11E2	1.14	5.80E1	5.80E1	0	9.00E1	1.14
485	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.12E3	1.47E-2	2.29E1	2.29E1	0	2.11E5	1.47E-2
260	3.06E3	3.42E-2	8.09E1	2.37E1	5.72E1	1.98E5	1.55E-2
300	2.71E3	1.45E-1	3.33E2	5.99E1	2.74E2	6.15E4	4.41E-2
340	2.05E3	1.88E-1	2.84E2	1.01E2	1.82E2	2.07E4	9.89E-2
380	1.38E3	2.81E-1	1.70E2	1.70E2	0	4.29E3	2.81E-1
420	6.14E2	7.81E-1	1.08E2	1.08E2	0	3.52E2	7.81E-1
460	2.52E2	6.76E-1	5.09E1	5.09E1	0	2.23E2	6.76E-1
485	0	0	0	0	0	0	0

Table 6-18
Calculated Mechanical Response of 10 Wt% Moisture in Cured Epoxy (T_g = 363K, t = 1 s)

Shear

T (K)	σ_b (bar)	γ_b	W_S (bar)	W_E (bar)	W_p (bar)	G_E (bar)	γ_E
220	1.58E3	2.24E-2	1.76E1	1.76E1	0	7.01E4	2.24E-2
260	1.58E3	1.02E-1	1.33E2	2.85E1	1.05E2	4.37E4	3.61E-2
300	1.50E3	4.33E-1	5.11E2	1.37E2	3.74E2	8.16E3	1.83E-1
340	1.14E3	6.78E-1	5.14E2	2.60E2	2.54E2	2.51E3	4.55E-1
380	7.87E2	1.05	2.98E2	2.98E2	0	5.38E2	1.05
420	4.32E2	1.24	8.89E1	8.89E1	0	1.16E2	1.24
460	7.79E1	9.04E-1	2.41E1	2.41E1	0	5.89E1	9.04E-1
468	0	0	0	0	0	0	0

Tension

T (K)	S_b (bar)	ϵ_b	W_T (bar)	W_E (bar)	W_p (bar)	E_E (bar)	ϵ_E
220	3.11E3	1.47E-2	2.28E1	2.28E1	0	2.10E5	1.47E-2
260	3.05E3	4.92E-2	1.19E2	2.93E1	8.94E1	1.54E5	1.95E-2
300	2.54E3	1.79E-1	3.79E2	7.62E1	3.03E2	4.22E4	6.01E-2
340	1.74E3	3.15E-1	4.10E2	1.36E2	2.74E2	1.10E4	1.57E-1
380	9.93E2	5.85E-1	2.48E2	2.48E2	0	1.45E3	5.85E-1
420	4.87E2	7.74E-1	8.53E1	8.53E1	0	2.84E2	7.74E-1
460	1.03E2	5.08E-1	2.01E1	2.01E1	0	1.56E2	5.09E-1
468	0	0	0	0	0	0	0

AD-A127 721 CAD/CAM HANDBOOK FOR POLYMER COMPOSITE RELIABILITY VOLUME II(U) ROCKWELL INTERNATIONAL THOUSAND OAKS CA SCIENCE CENTER D H KAELBLE MAR 83 SC5291.7FR-VOL-2 2/3

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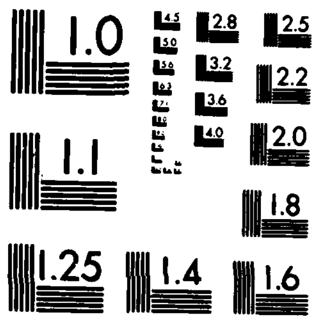

MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

Table 6-19
Relations Between English and SI Units in The Composite Fracture Energy and Strength Model

Input Variable	English Units	SI Units
D, V	2E-4 in, 0.5	5.08E-6m, 0.5
E, S	1E7 psi, 4E5 psi	6.89E10 N/m^2, 2.76E9N/m^2
G, L	5E5 psi, 5E3 psi	3.44E9N/m^2, 3.44E7N/m^2
Y, YY	1E6 psi, 1E4 psi	6.89E9N/m^2, 6.89E7N/m^2
LB, LF	5E3 psi, 5E2 psi	3.44E7N/m^2, 3.44E6N/m^2
Output (1)		
Inter-fiber Spacing	(in.) = 1.7E-4	(m) = 4.30E-6
Shear Stress Conc.	$(in.)^{-1}$ = 4360	$(m)^{-1}$ = 1.71E5
Max. F-M Bond St.	(psi) = 8.7E5	(N/m^2) = 6.01E8
F-M Debond Length	(in.) = 3.7E-3	(m) = 9.61E-4
Inter. Shear St.	(psi) = 5000	(N/m^2) = 3.44E7
Comp. Tens. Mod.	(psi) = 5.5E6	(N/m^2) = 3.79E10
Comp. Tens. St.	(psi) = 1.04E5	(N/m^2) = 7.18E8
Crit. Crack Length	(in.) = 7.5E-3	(m) = 1.92E-3
Output (2)		
Unflawed St. (min)	(psi) = 6.11E4	(N/m^2) = 4.2E8
Unflawed St. (max)	(psi) = 1.76E4	(N/m^2) = 1.22E9
Crit. Stress Int (min)	$(lb^2/in.^3)^{1/2}$ = 9406	$(N^2/m^3)^{1/2}$ = 3.27E7
Crit. Stress Int (max)	$(lb^2/in.^3)^{1/2}$ = 2.7E4	$(N^2/m^3)^{1/2}$ = 9.47E7
Output (3)		
F-M Bond Stress	(psi) = 5000	(N/m^2) = 3.44E7
Fiber (W_{Fb}/A)	(lb/in.) = 1.67	(N/m) = 2.95E3
Matrix (W_{Sb}/A)	(lb/in.) = 14.4	(N/m) = 2.53E4
Frict. (W_{Fb}/A)	(lb/in.) = 118	(N/m) = 2.08E5
Tot. (W_b/A)	(lb/in.) = 134	(N/m) = 2.36E5
Crit. Length (L_c)	(in.) = 7.54E-3	(m) = 1.92E-3

Table 6-20

First Estimate of Composite Fracture Energy and Strength (English Units, LB = 5000 psi, LF = 500 psi)

```
FIBER DIAMETER(D), VOLUME FRACTION(V)= 2E-04  .5
FIBER TENSILE MODULUS(E), STRENGTH(S)= 1E+07  400000
MATRIX SHEAR MODULUS(G), STRENGTH(L)= 500000  5000
MATRIX TENSILE(Y), STRENGTH(YY)= 1E+06  10000
F-M BOND STRENGTH(LB), FRICT. STRENGTH(LF)= 5000  500

INTER-FIBER SPACING(R1)= 1.69212E-04
SHEAR STRESS CONC.(A)= 4360.29
MAX. F-M BOND STRENGTH(LM)= 87205.7
F-M DEBOND LENGTH(BL)= .0377066
INTERLAM. SHEAR STRENGTH(IL)= 5000
COMPOSITE TENSILE MODULUS= 5.5E+06
COMPOSITE CONTINUUM TENSILE STRENGTH= 104055
CRITICAL CRACK LENGTH= .0754131
TO CONTINUE PRESS ENTER? _


             FRACTURE MECHANICS ANALYSIS
UNFLAWED STRENGTH (MIN.)= 61114.4 (MAX.)= 176749
CRIT. STRESS INTENSITY (MIN.)= 29746.9 (MAX.)= 86031.3
FLAW SIZE          CRACK LENGTH     MIN. STRENGTH      MAX  STRENGTH
 .0753959           4.71332E-03      61121.3            176769
 .0752844           9.42664E-03      61166.6            176900
 .0745363           .0188533         61472.8            177786
 .0709825           .0377065         62992.8            182182
 .0754131           .0754131         61114.4            176749
 .150801            .150826          43218              124991
 .301652            .301652          30557.2            88374.6
 .603304            .603304          21607.2            62490.3
 1.20661            1.20661          15278.6            44187.3
 2.41322            2.41322          10803.6            31245.2
 TO CONTINUE PRESS ENTER? _


             FRACTURE WORK PER UNIT CROSSECTION AREA
 F-M BOND   FIBER      MATRIX     FRICT.     TOTAL      CRIT.FIBER
 STRESS     WORK       WORK       WORK       WORK       LENGTH
  5000       16.7585    144.129    1184.82    1345.71    .0754131
 PRESS ENTER TO CONTINUE?
  0          17.7778    0          1333.33    1351.11    .08
  9689.53    15.8025    263.374    1053.5     1332.67    .0711111
  19379.1    13.8272    460.905    806.584    1281.32    .0622222
  29068.6    11.8519    592.593    592.593    1197.04    .0533333
  38758.1    9.87654    658.436    411.523    1079.84    .0444444
  48447.6    7.90124    658.436    263.375    929.712    .0355556
  58137.2    5.92592    592.593    148.148    746.667    .0266667
  67826.7    3.95062    460.905    65.8436    530.7      .0177778
  77516.2    1.97531    263.374    16.4609    281.811    8.88889E-03
  87205.7    0          0          0          0          0
  PRESS ENTER TO CONTINUE? _
```

Table 6-21

Second Estimate of Composite Fracture Energy and Strength
(English Units, LB = 5000 psi, LF = 5000 psi)

```
FIBER DIAMETER(D), VOLUME FRACTION(V)= 2E-04  .5
FIBER TENSILE MODULUS(E), STRENGTH(S)= 1E+07  400000
MATRIX SHEAR MODULUS(G), STRENGTH(L)= 500000  5000
MATRIX TENSILE(Y), STRENGTH(YY)= 1E+06  10000
F-M BOND STRENGTH(LB), FRICT. STRENGTH(LF)= 5000  5000

INTER-FIBER SPACING(Ri)= 1.69212E-04
SHEAR STRESS CONC.(A)= 4360.29
MAX. F-M BOND STRENGTH(LM)= 87205.7
F-M DEBOND LENGTH(BL)= 3.77066E-03
INTERLAM. SHEAR STRENGTH(IL)= 5000
COMPOSITE TENSILE MODULUS= 5.5E+06
COMPOSITE CONTINUUM TENSILE STRENGTH= 104055
CRITICAL CRACK LENGTH= 7.54131E-03
TO CONTINUE PRESS ENTER? _

            FRACTURE MECHANICS ANALYSIS
UNFLAWED STRENGTH (MIN.)= 61114.4 (MAX )= 176749
CRIT. STRESS INTENSITY (MIN.)= 9406 81 (MAX.)= 27205.5
FLAW SIZE        CRACK LENGTH    MIN  STRENGTH    MAX. STRENGTH
 7.53959E-03      4.71332E-04     61121 4          176770
 7.52844E-03      9.42664E-04     61166 6          176900
 7.45363E-03      1.88533E-03     61472 8          177786
 7.09825E-03      3.77065E-03     62992 8          182182
 7.54131E-03      7.54131E-03     61114 4          176749
 .0150801         .0150826        43218            124991
 .0301652         .0301652        30557 2          88374.7
 .0603304         .0603304        21607 2          62490.4
 .120661          .120661         15278 6          44187.4
 .241322          .241322         10803 6          31245.2
TO CONTINUE PRESS ENTER? _

            FRACTURE WORK PER UNIT CROSSECTION AREA
F-M BOND   FIBER      MATRIX     FRICT.     TOTAL      CRIT.FIBER
STRESS     WORK       WORK       WORK       WORK       LENGTH
 5000       1.67585    14.4129    118.482    134.571    7.54131E-03
PRESS ENTER TO CONTINUE?
 0          1.77778    0          133.333    135.111    8E-03
 9689.53    1.58025    26.3375    105.35     133.267    7.11111E-03
 19379.1    1.38272    46.0905    80.6584    128.132    6.22222E-03
 29068.6    1.18519    59.2593    59.2593    119.704    5.33333E-03
 38758.1    .987654    65.8436    41.1523    107.984    4.44444E-03
 48447.6    .790124    65.8436    26.3375    92.9712    3.55556E-03
 58137.2    .592593    59.2592    14.8148    74.6667    2.66667E-03
 67826.7    .395062    46.0905    6.58437    53.07      1.77778E-03
 77516.2    .197531    26.3374    1.64609    28.1811    8.88889E-04
 87205 7    0          0          0          0          0
PRESS ENTER TO CONTINUE? _
```

Table 6-22

Relations Between English and SI Units in the Peel Mechanics Model

Input Variable	English Units	SI Units
H, A	1E-3 in., 8E-3 in.	2.54E-5m, 2.03E-4m
B, E	1.0 in., 1E4 psi	2.54E-2m, 6.89E7 N/m^2
Y, SA	5E4 psi, 2E4 psi	3.45E8m, 1.38E8N/m^2
G, LA	1.67E4 psi, 6.67E3 psi	1.15E8N/m^2, 4.60E7 N/m^2
Output (1)		
Cleavage Stress Conc.	($in.^{-1}$) = 6.95E2	(m^{-1}) = 2.74E4
Shear Stress Conc.	($in.^{-1}$) = 3.23E2	(m^{-1}) = 1.27E4
180 Deg. Radius of Curv.	(in.) = 3.22E-4	(m) = 8.209E-6
0 Deg. Peel Force	(lb) = 20.6	(N) = 91.8
180 Deg. Peel Force	(lb) = 16.0	(N) = 71.2
Output (2)		
Peel Angle	(deg) = 177.9	(deg) = 177.9
Peel Work	(lb/in.) = 35.2	(N/m) = 6.16E3
Peel Force	(lb) = 14.8	(N) = 65.8
K	.963	.963
Tensile Stress	(psi) = 2E4	(N/m^2) = 1.38E8
Shear Stress	(psi) = -4.79E3	(N/m^2) = -3.30E7

Table 6-23
First Estimate of Laminate Peel and Shear Properties
(Flexible Adherend Tensile Modulus = 1E4 psi, English Units)

```
RIBBON HALF THICKNESS(H), ADHESIVE THICKNESS(A)? .001,.008
BOND WIDTH(B), RIBBON   TENSILE MODULUS(E)? 1,1E4
ADHESIVE TENSILE MODULUS(Y),STRENGTH(SA)? 5E4,2E4
ADHESIVE SHEAR MODULUS(G),STRENGTH(LA)? 1.67E4,6.67E3
CLEAVAGE STRESS CONC.(BA)= 695.789
SHEAR STRESS CONC.(GA)= 323.071
180 DEG. RAD. OF CURV.(R)= 3.22749E-04
0 DEG. PEEL FORCE(PS)= 20.6456
180 DEG. PEEL FORCE(PC)= 16
```

PEEL ANGLE	PEEL WORK	PEEL FORCE	K	TENSILE STRESS	SHEAR STRESS
177.943	35.1768	14.8403	.962936	20000	-4791.38
147.943	17.0924	8.31579	.692002	20000	-2276.95
117.944	11.5577	7.02803	.567962	20000	-1064.12
87.9443	8.67872	7.58096	.476341	20000	87.2691
77.9462	8.06533	8.11386	.447893	20000	547.412
67.9481	7.65196	9.00554	.419243	20000	1092.33
57.95	7.53574	10.35	.389619	20000	1774.4
47.9519	7.96186	12.424	.358076	20000	2688.27
37.9538	9.59627	15.8136	.323288	20000	4028.42
32.9542	11.4109	18.3874	.304058	20000	4984.66
27.9546	14.6422	21.9796	.283097	20000	6272.44
22.955	14.3437	22.4215	.279083	16801.5	6670
17.9553	12.8328	21.7033	.280759	12948.7	6670
12.9557	11.7599	21.1855	.281979	9210.26	6670
7.9561	11.0640	20.8462	.282074	5598.38	6670

Table 6-24

Second Estimate of Laminate Peel and Shear Properties
(Flexible Adherend Tensile Modulus = 5E4 psi, English Units)

RIBBON HALF THICKNESS(H), ADHESIVE THICKNESS(A)? .001, .008
BOND WIDTH(B), RIBBON TENSILE MODULUS(E)? 1,5E4
ADHESIVE TENSILE MODULUS(Y),STRENGTH(SA)? 5E4,2E4
ADHESIVE SHEAR MODULUS(G),STRENGTH(LA)? 1.67E4,6.57E3
CLEAVAGE STRESS CONC.(BA)= 465.303
SHEAR STRESS CONC.(GA)= 144.482
180 DEG. RAD. OF CURV.(R)= 7.21688E-04
0 DEG. PEEL FORCE(PS)= 46.165
180 DEG. PEEL FORCE(PC)= 16

PEEL ANGLE	PEEL WORK	PEEL FORCE	K	TENSILE STRESS	SHEAR STRESS
177.943	31.5538	15.2039	.974606	20000	-2195.2[illegible]
147.943	18.7644	9.89172	.755712	20000	-121[illegible] 2[illegible]
117.944	13.3668	8.83588	.6368	20000	-598 [illegible]
87.9443	9.94176	9.81231	.543725	20000	50.85[illegible]
77.9462	9.82199	10.6822	.513914	20000	322 30[illegible]
67.9481	8.19742	11.9760	.483483	20000	649 68[illegible]
57.95	7.49303	13.9051	.451604	20000	1066.1[illegible]
47.9519	6.99257	16.8666	.417214	20000	1632 14
37.9538	6.94726	21.7879	.378777	20000	2473 07
32.9542	7.30912	25.3918	.357308	20000	3073 33
27.9546	8.22931	30.3457	.333734	20000	3893.35
22.955	10.307	38.1692	.307336	20000	5073 06
17.9553	14.1381	48.5277	.280809	19354.7	6670
12.9557	12.4262	47.3715	.282006	13769 4	6670
7.9561	11.3131	46.6142	.282796	8377	6670

Table 6-25

Third Estimate of Laminate Peel and Shear Properties
(Flexible Adherend Tensile Modulus = 2.5E5 psi, English Units)

```
RIBBON HALF THICKNESS(H), ADHESIVE THICKNESS(A)? .001, .008
BOND WIDTH(B), RIBBON   TENSILE MODULUS(E)? 1, 2.5E5
ADHESIVE TENSILE MODULUS(Y),STRENGTH(SA)? 5E4,2E4
ADHESIVE SHEAR MODULUS(G),STRENGTH(LA)? 1.67E4,6.67E3
CLEAVAGE STRESS CONC.(BA)= 311.166
SHEAR STRESS CONC.(GA)= 64.6142
180 DEG. RAD. OF CURV.(R)= 1.61374E-03
0 DEG. PEEL FORCE(PS)= 103.228
180 DEG. PEEL FORCE(PC)= 16
```

PEEL ANGLE	PEEL WORK	PEEL FORCE	K	TENSILE STRESS	SHEAR STRESS
177.943	31.1472	13.4591	.982733	20000	-998.235
147.943	21.2076	11.4085	.811585	20000	-624.753
117.944	15.9552	10.7849	.703537	20000	-326.554
87.9443	12.1653	12.4569	.612631	20000	28.8703
77.9462	11.0442	13.7214	.582451	20000	185.146
67.9481	9.96251	15.5635	.551143	20000	377.556
57.95	8.91483	18.2822	.517826	20000	626.859
47.9519	7.91709	22.4474	.481313	20000	971.426
37.9538	7.04729	29.2705	.439834	20000	1491.29
32.9542	6.73657	34.4802	.416371	20000	1869.45
27.9546	6.62322	41.7936	.390373	20000	2385.37
22.955	6.94244	52.6562	.360970	20000	3132.91
17.9553	8.34284	70.178	.326816	20000	4313.65
12.9557	13.0984	102.425	.285449	20000	6449.67
7.9561	11.8676	104.232	.282823	12523.8	6670

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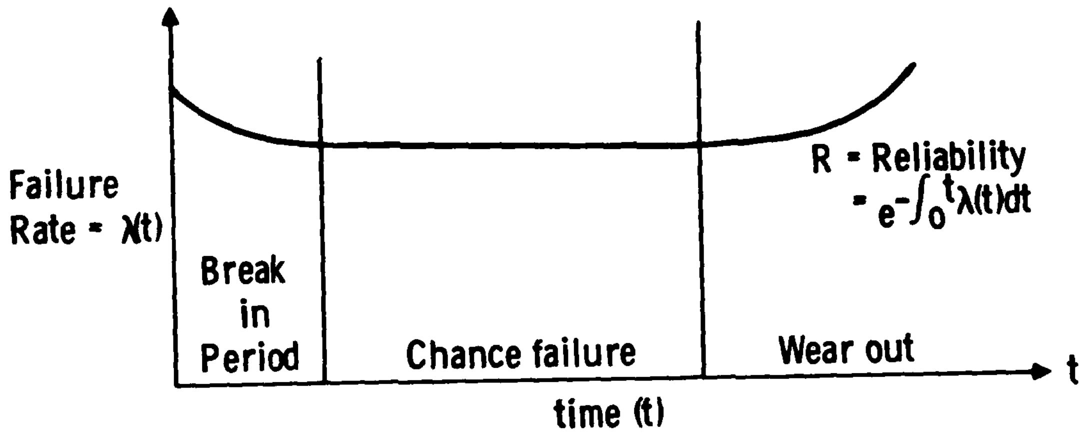

Fig. 1-1 Failure rate criteria for reliability.

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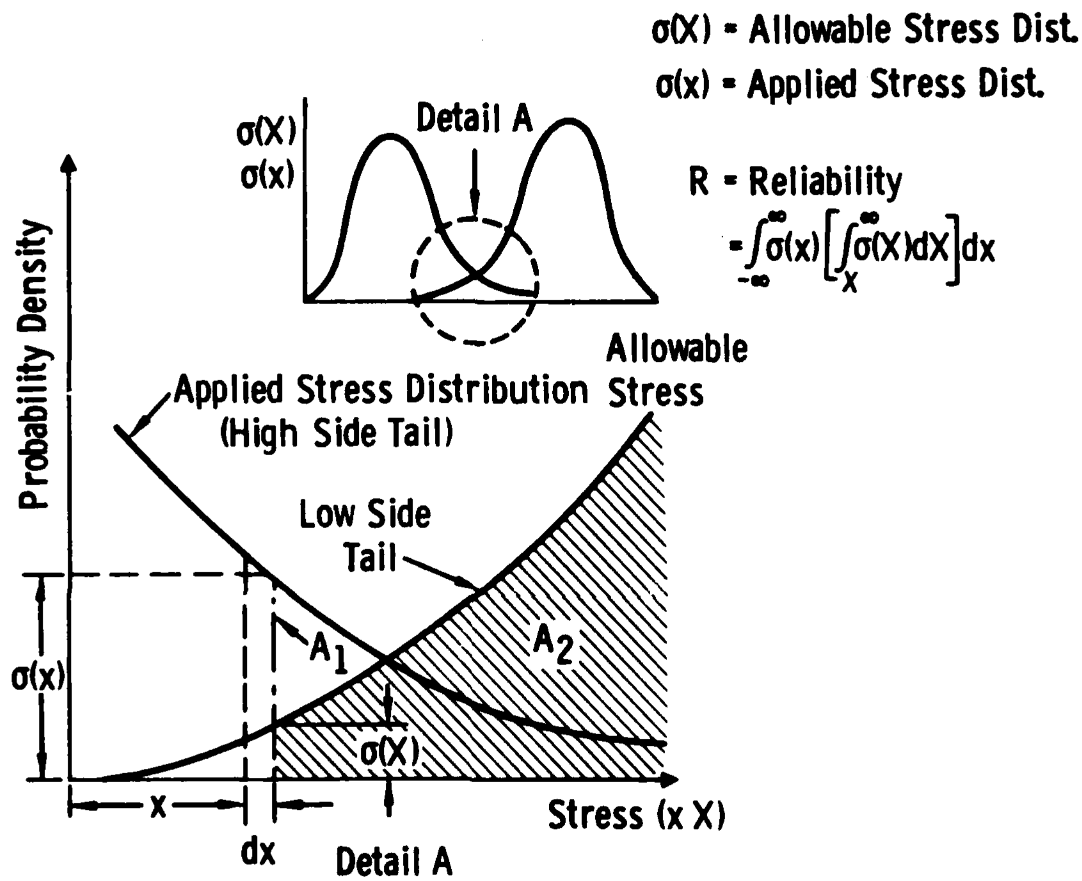

Fig. 1-2 Applied and allowable stress distribution analysis of reliability.

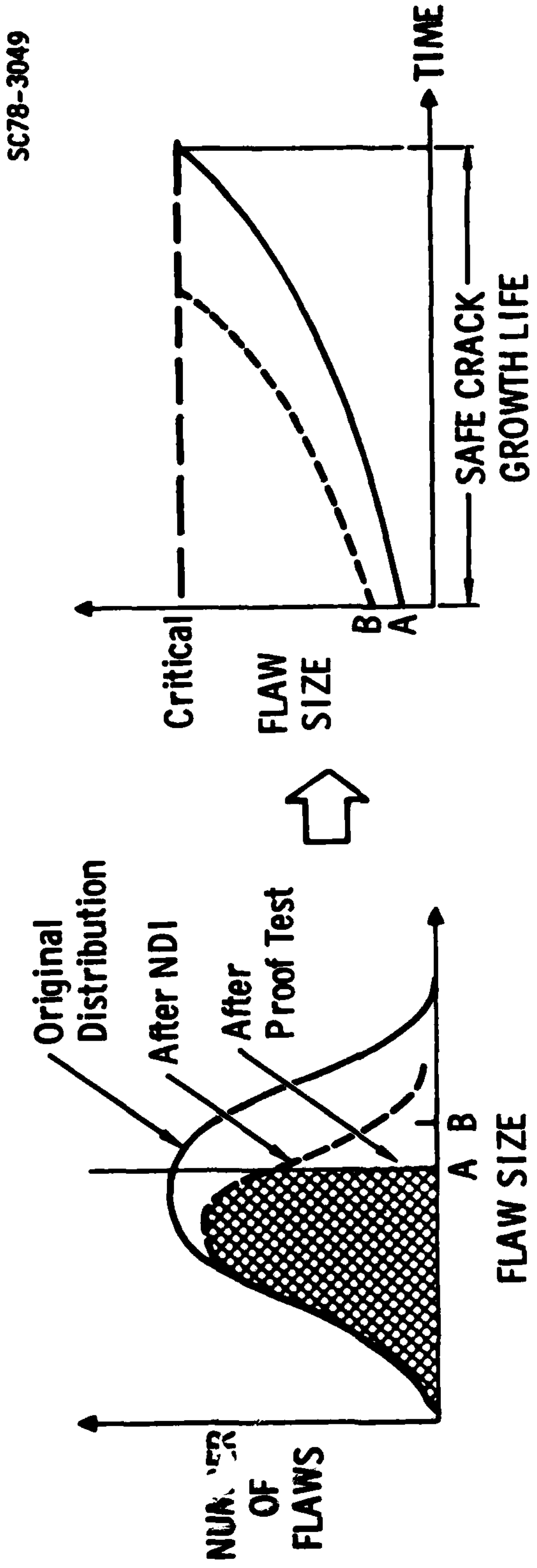

Fig. 1-3 Fracture mechanics criteria for structure reliability.

$$\text{RELIABILITY} = R = \exp\left[-V_i K_i N_i \left(\frac{\sigma}{\beta}\right)^m\right] \qquad \frac{\beta_j}{\beta_i} = \left[\frac{V_i\ K_i\ N_i}{V_j\ K_j\ N_j}\right]^{1/m}$$

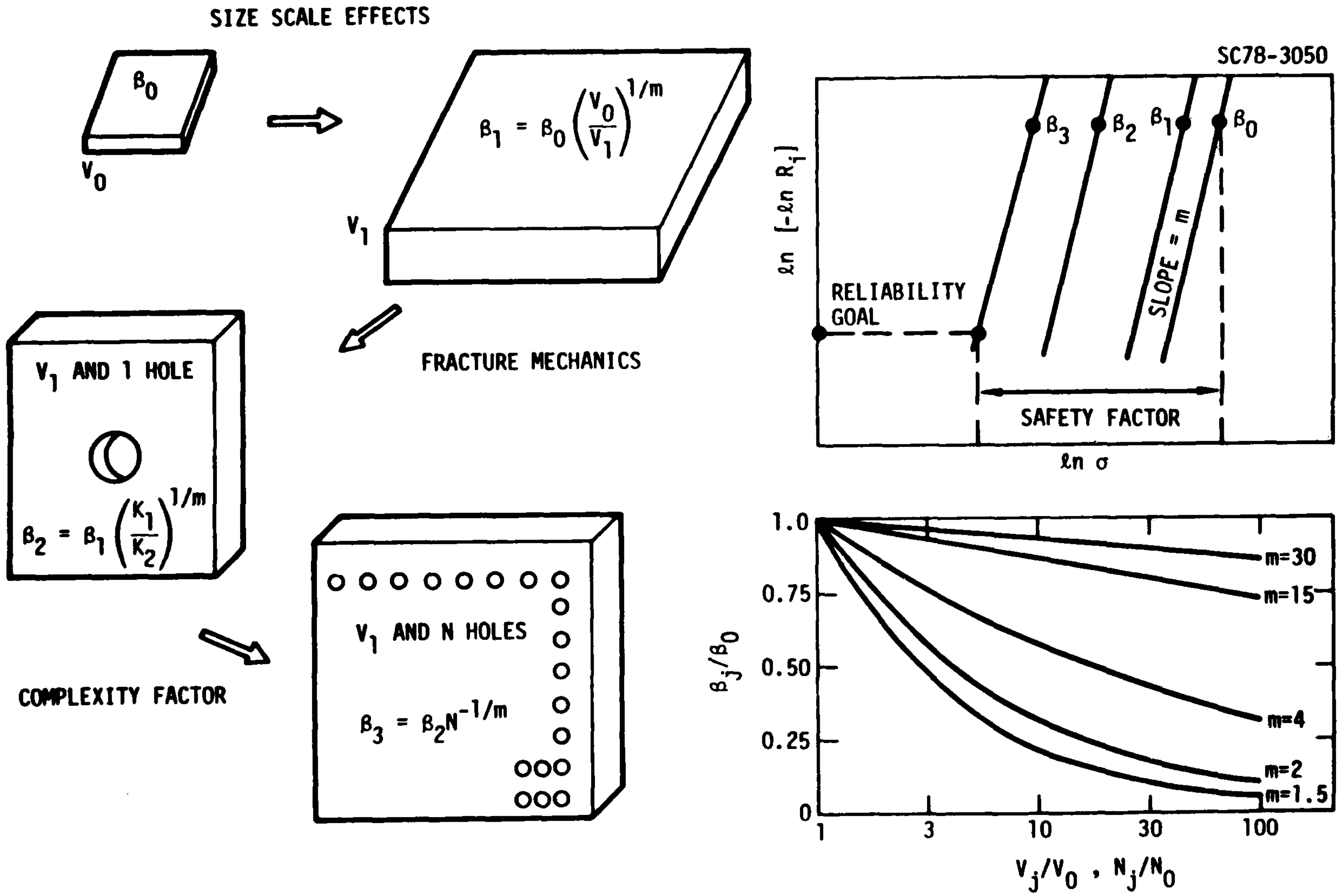

Fig. 1-4 Weibull criteria for structure reliability.

SC78-3051

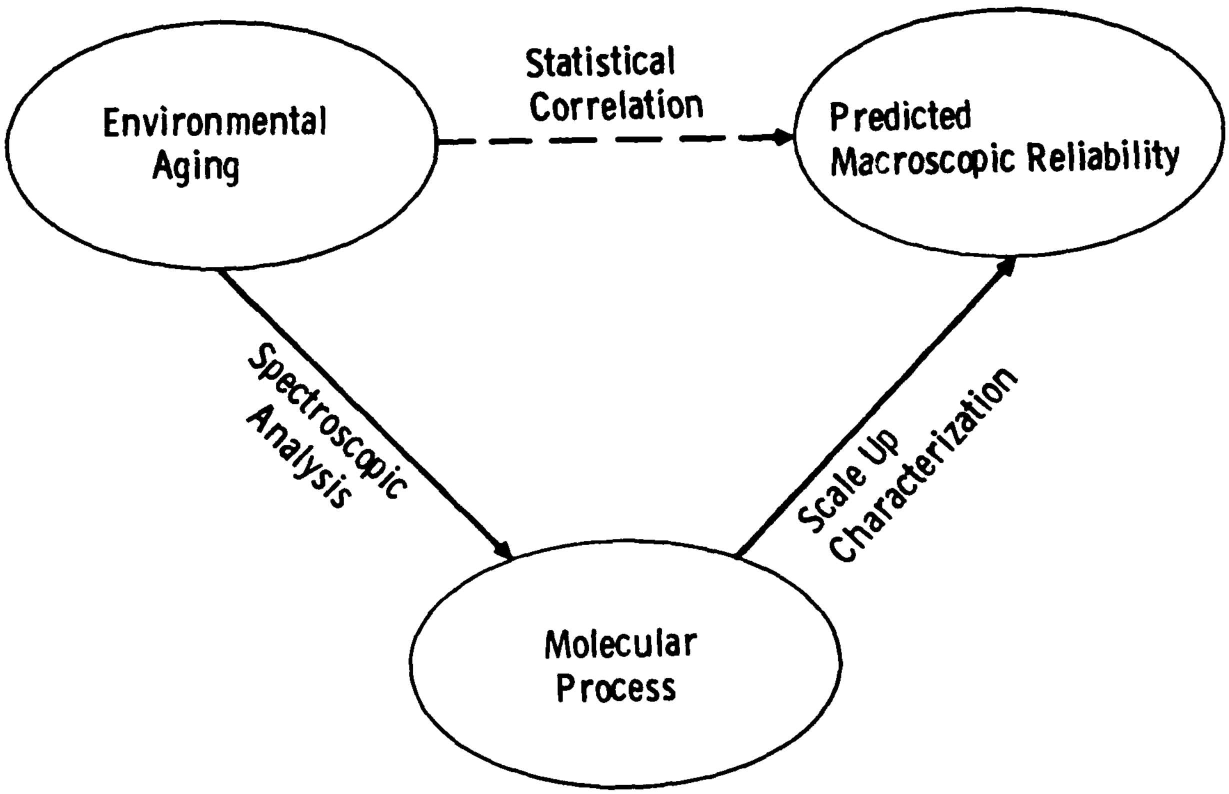

Fig. 1-5 Preferred dual path for correlating environmental aging with macroscopic strength.

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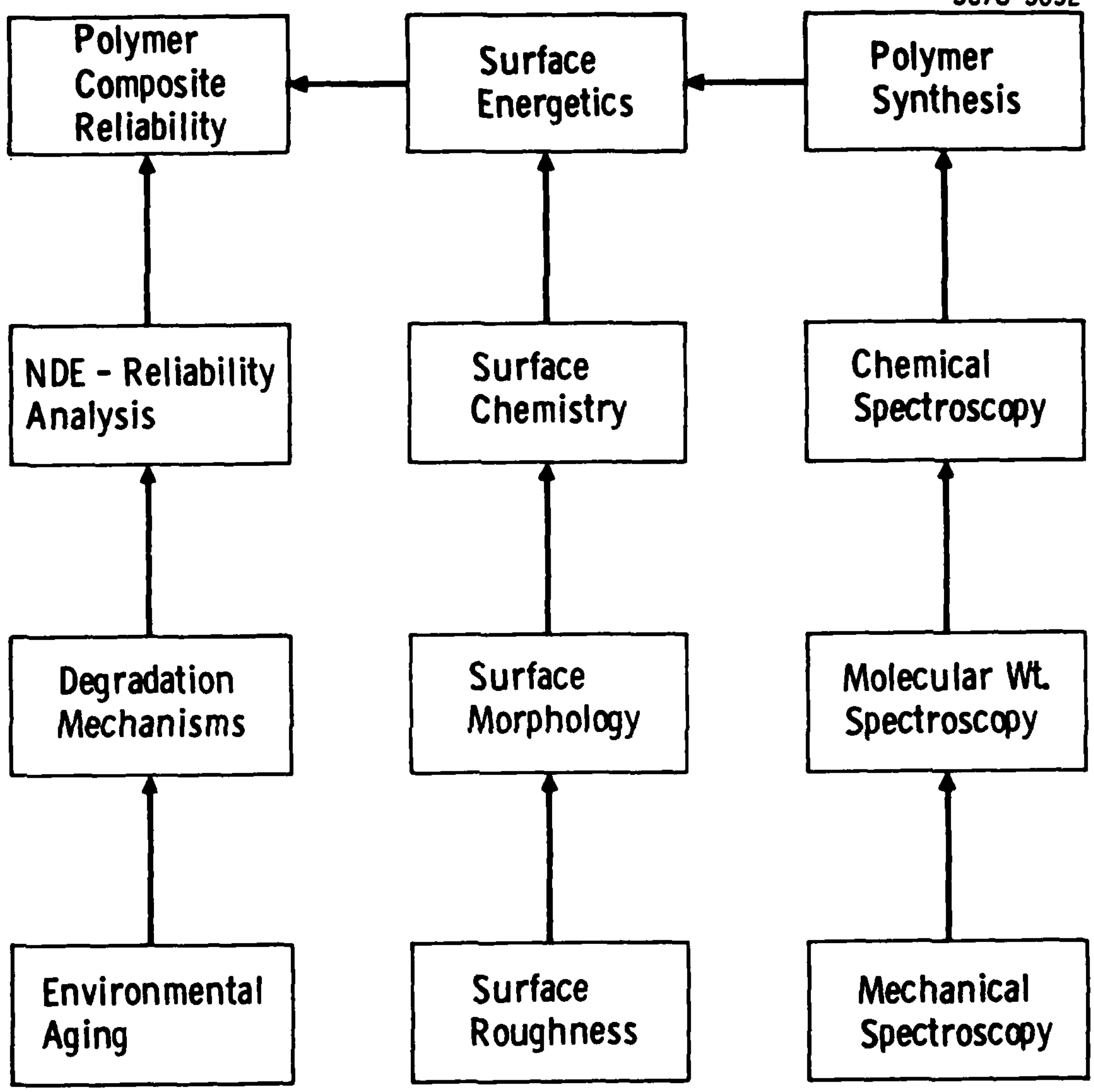

Fig. 1-6 Technical approach to polymer composite reliability.

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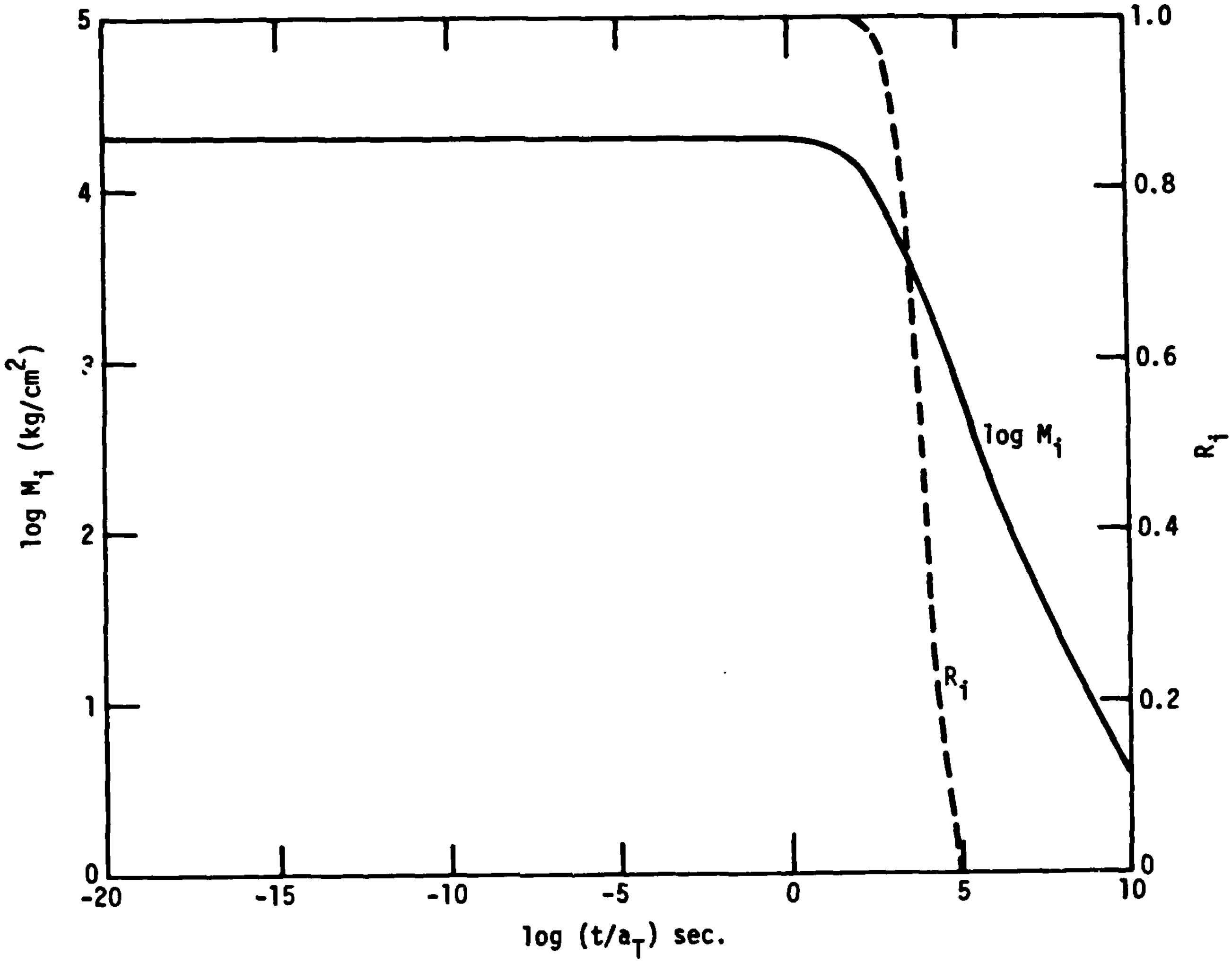

Fig. 1-7 Calculated function of M_i and R_i for M_o = 20,000 kg/cm^2, M_∞ = 2.0 kg/cm^2, τ = 100 s, R_∞ = 0, τ_o = 10^4 s, m = 1.0.

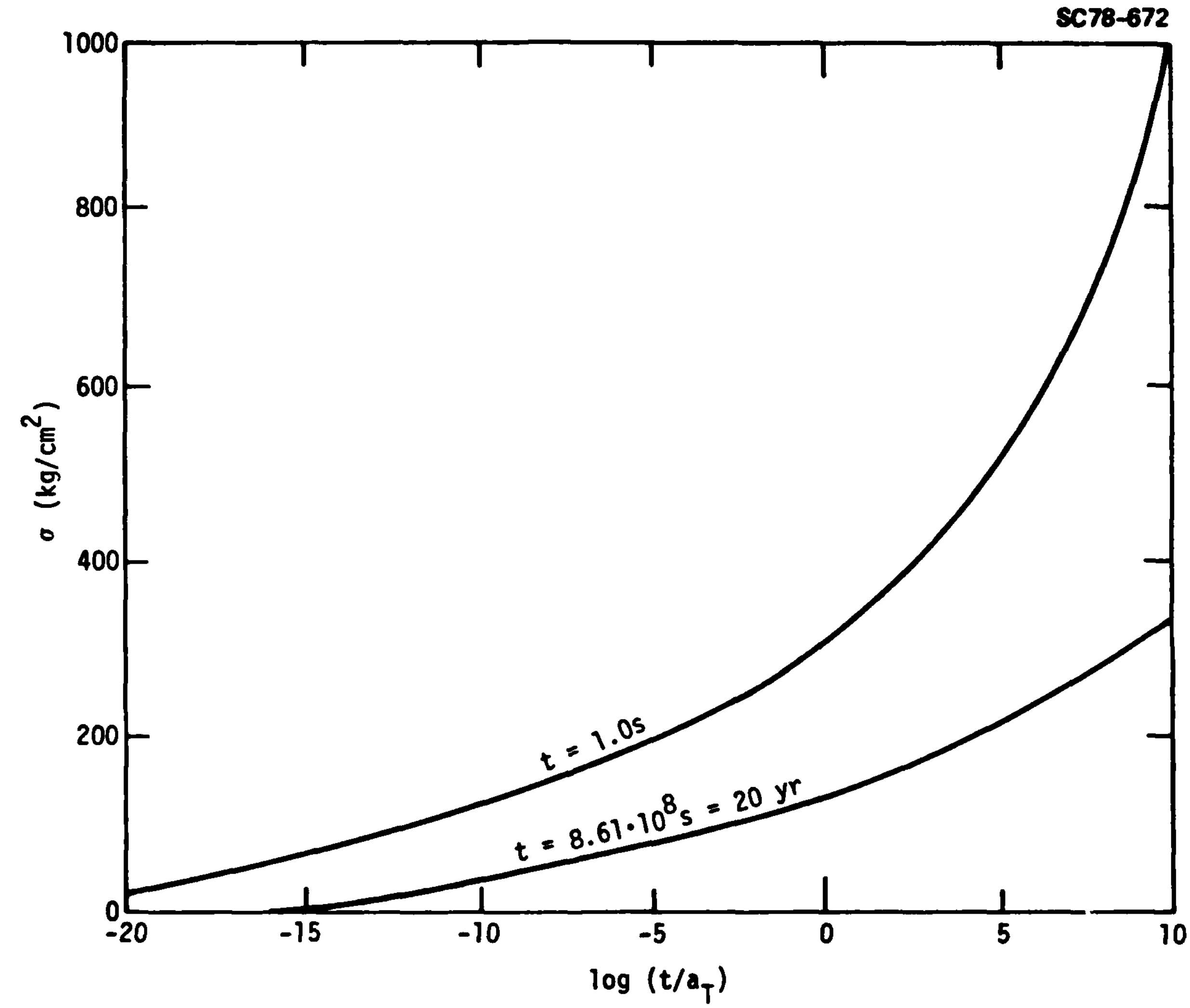

Fig. 1-8 Illustrative relations between tensile stress σ and time shift factor log (t/a_T).

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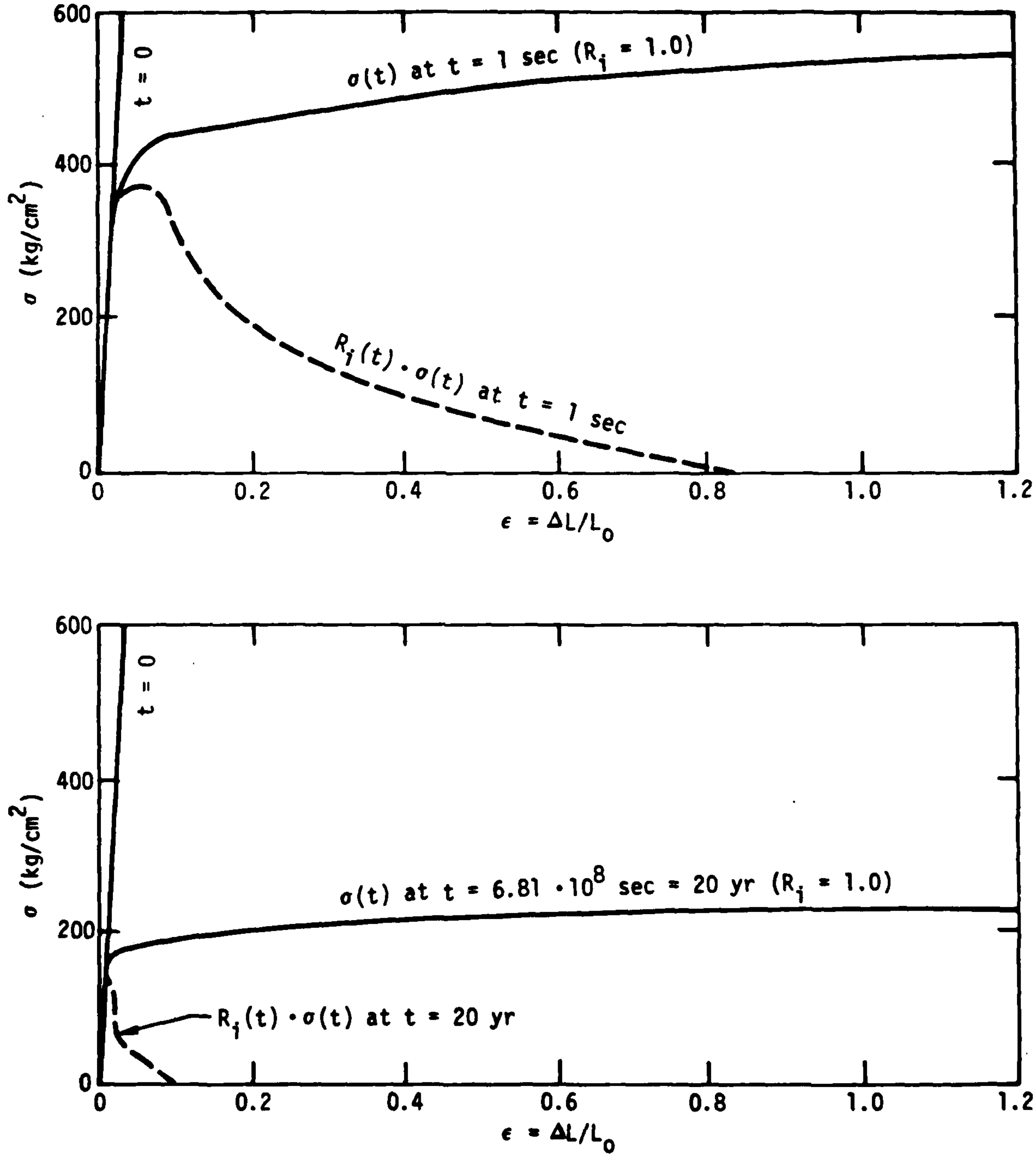


Fig. 1-9 Calculated tensile creep stress $\sigma(t)$ vs strain $\varepsilon(t)$ (solid curves) and reliability $R_i(t)$ reduced stress $R_i(t)*\sigma_i(t)$ vs strain $\varepsilon(t)$ (dashed curves) at t = 1 s (upper view) and t = 20 yr (lower view).

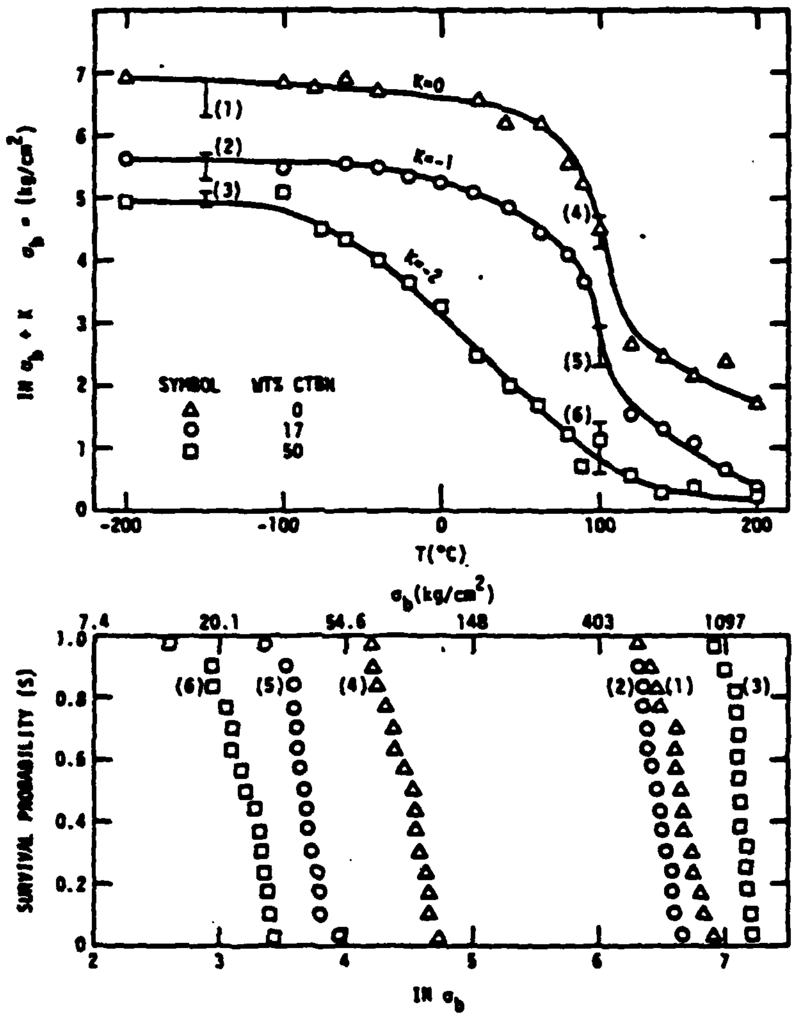


Fig. 1-10 (a) The temperature and composition dependence of the tensile strength for a rubber modified epoxy.
(b) The stress dependence of the survival probability for rubber modified epoxy at -150°C and 100°C.

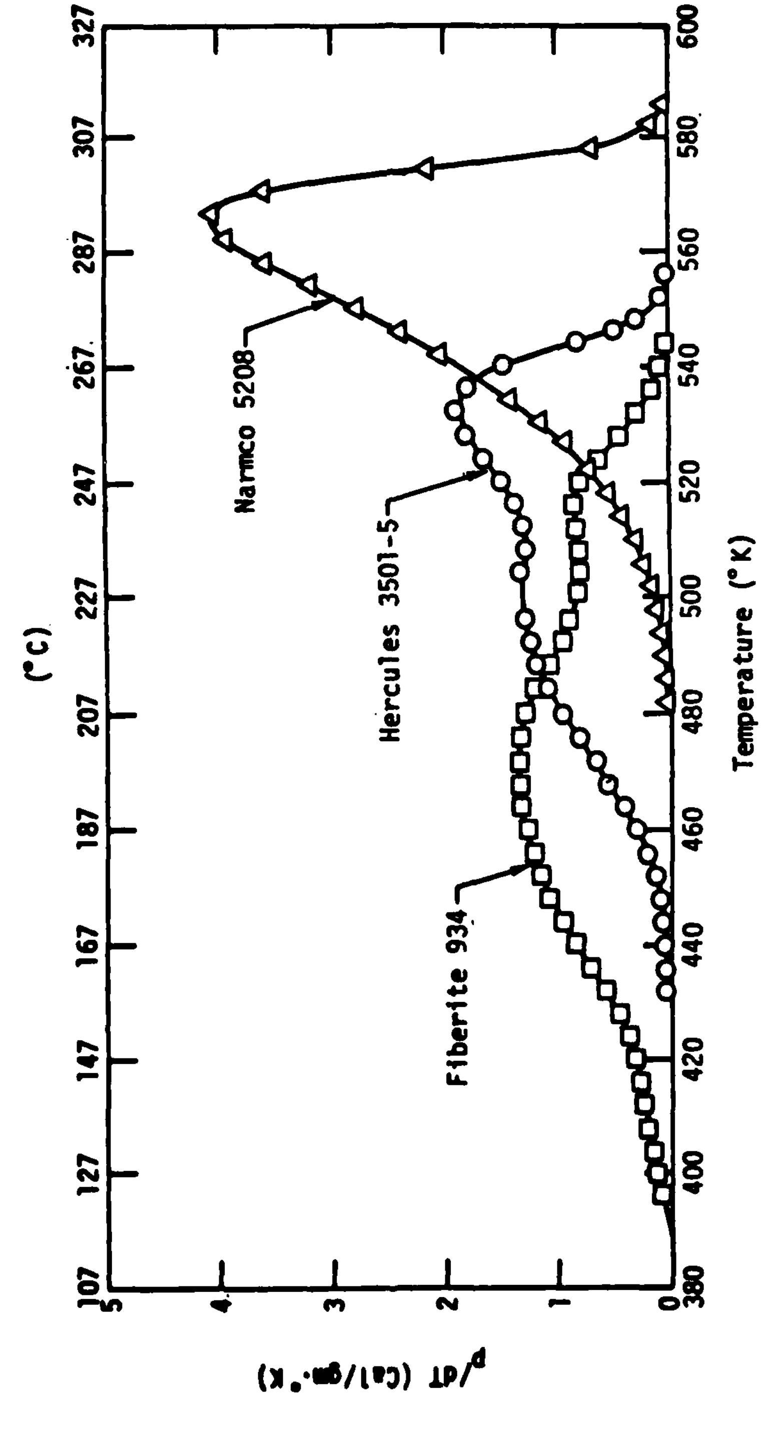


Fig. 1-11 DSC thermograms for curing reactions of commercial epoxy matrix materials extracted from prepreg (DSC scan rate ϕ = 20°C/min).

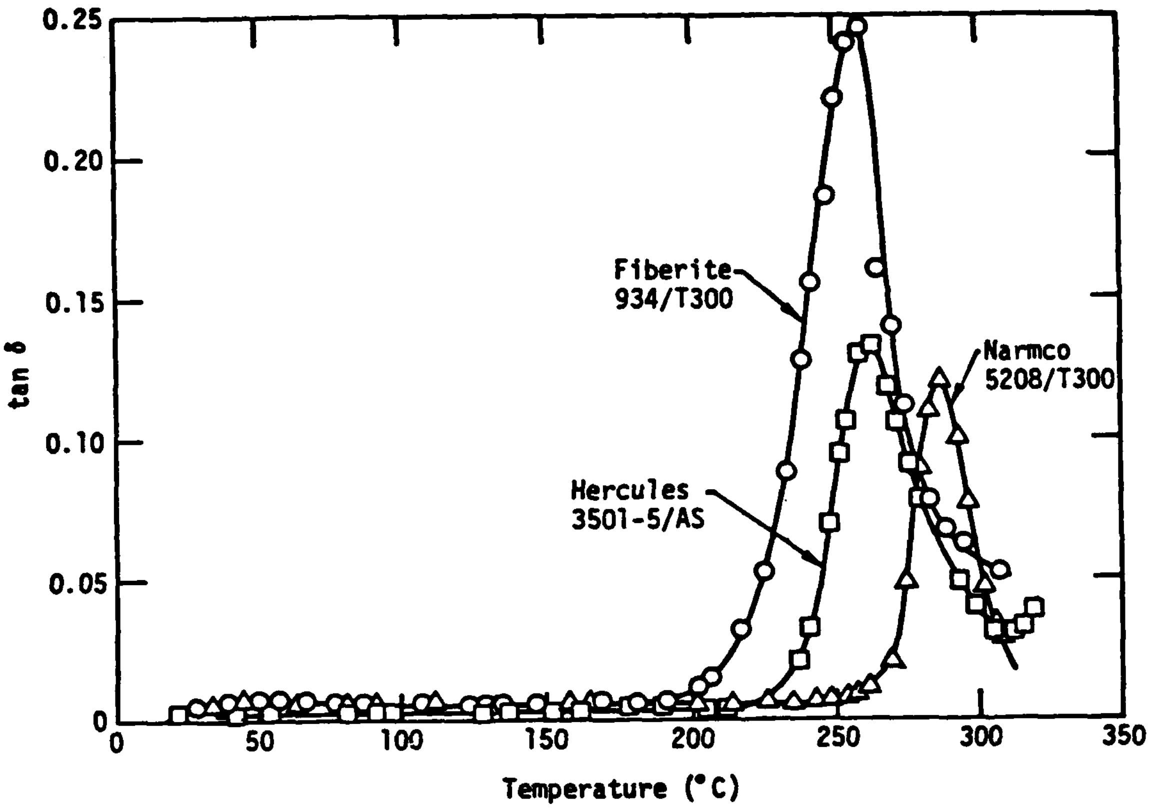


Fig. 1-12 Rheovibron thermal scans for flexural damping in cured reinforced graphite-epoxy composite in the dry unaged condition.

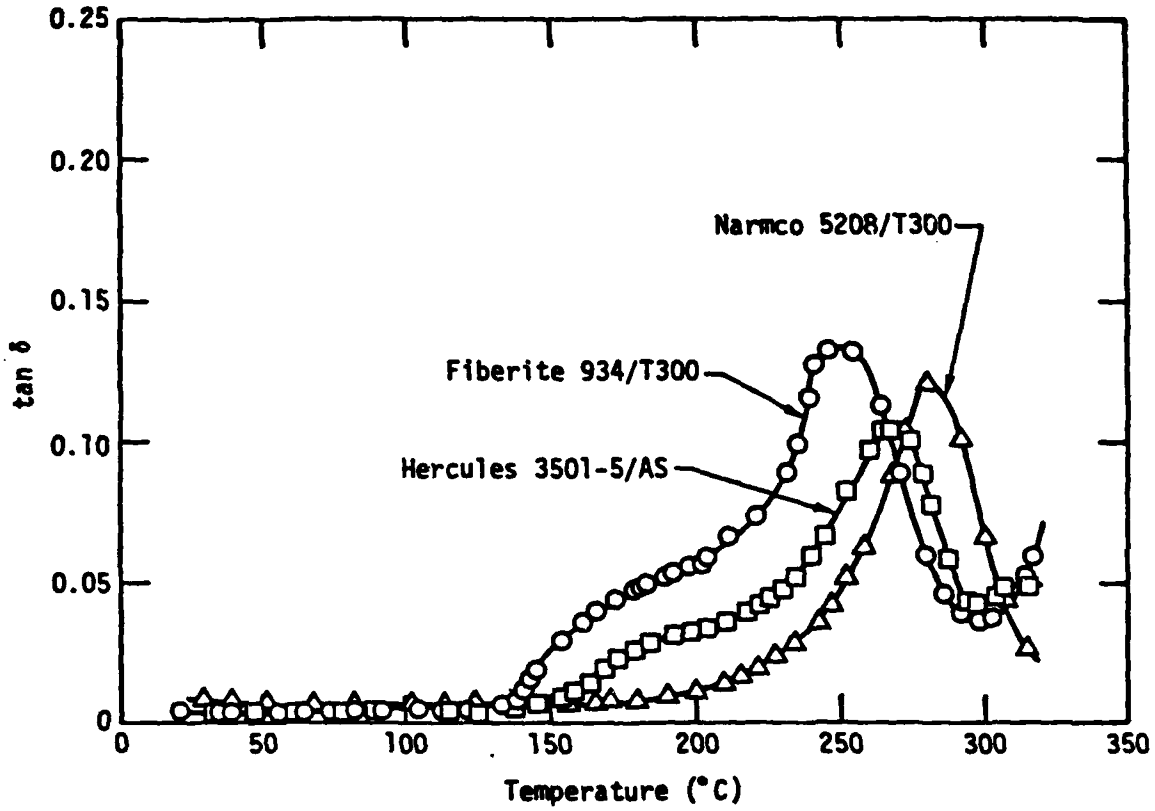


Fig. 1-13 Rheovibron thermal scans for flexural damping in cured uniaxial reinforced graphite-epoxy composite in the wet-aged condition.

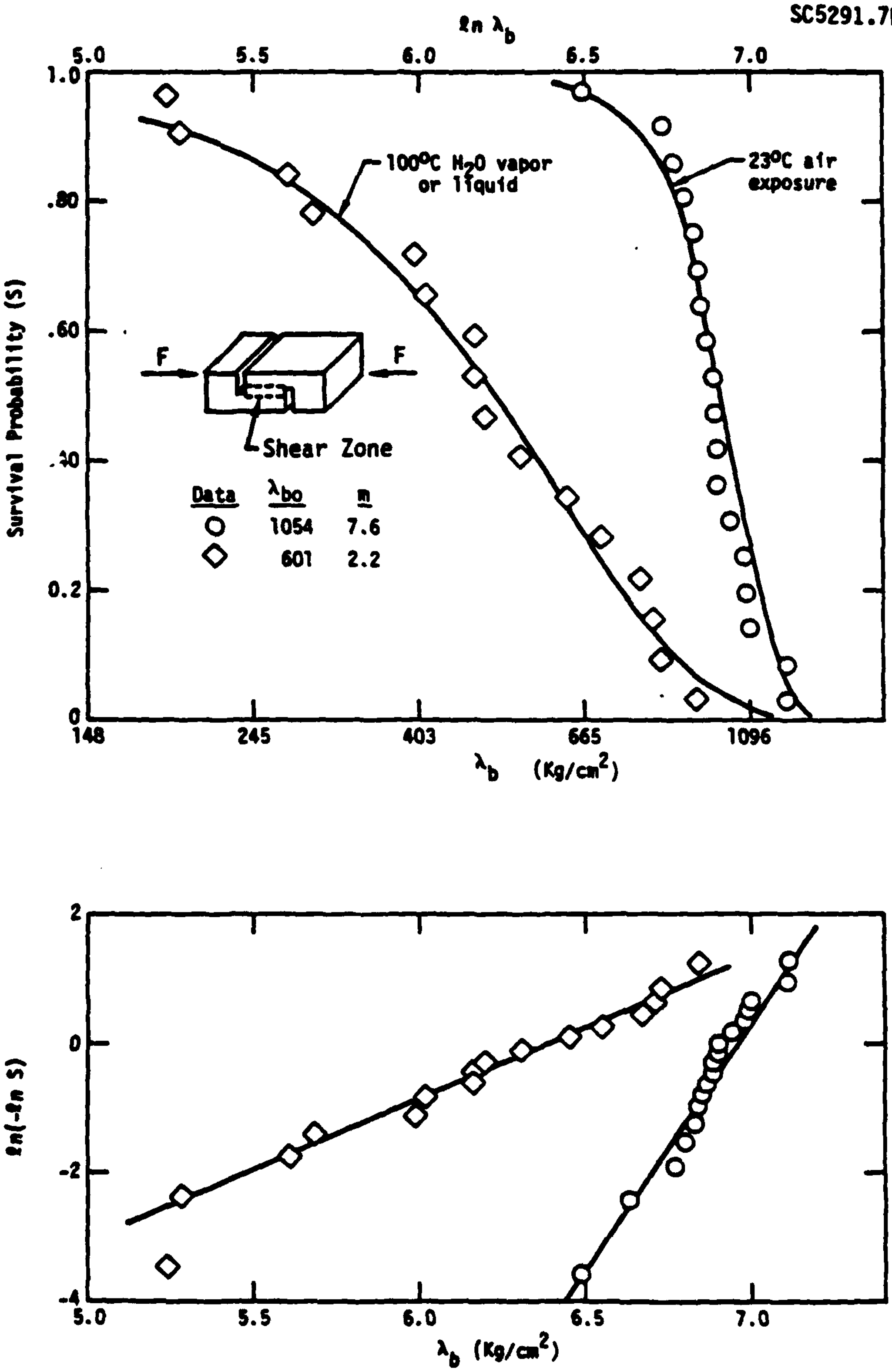


Fig. 1-14 Cumulative distribution function of survival probability.

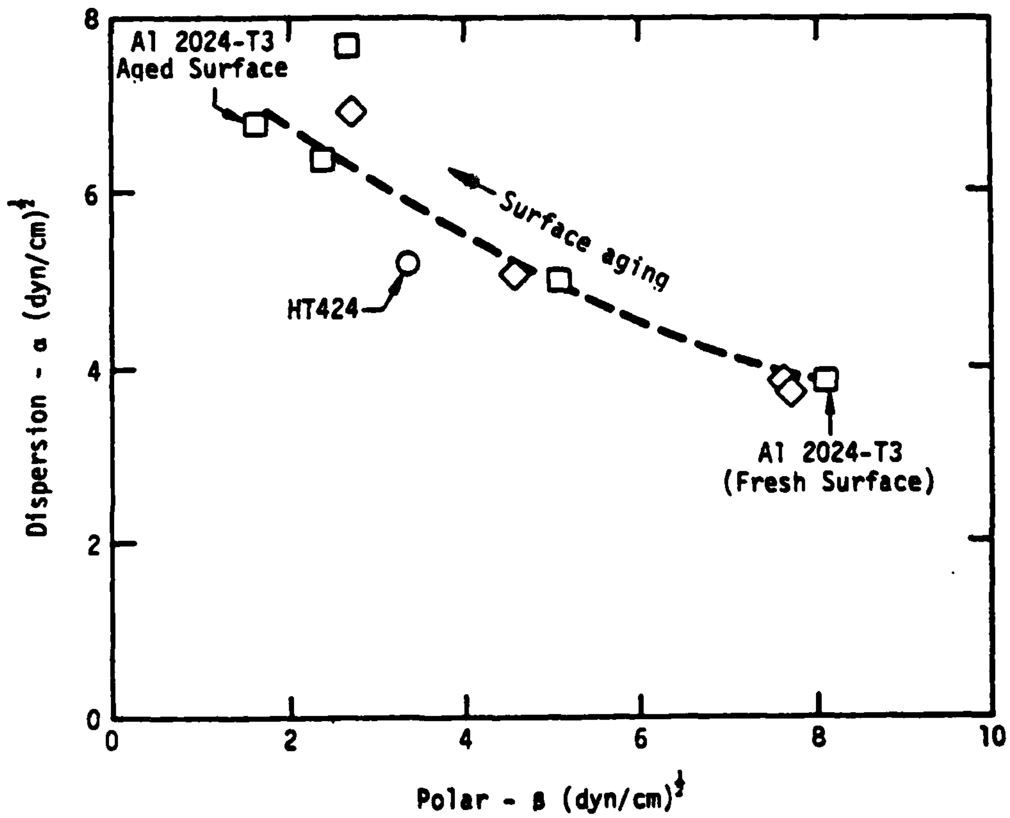


Fig. 1-15 Dispersion (α) and polar (β) components of the solid-vapor surface tension $\gamma_{SV} = \alpha^2 + \beta^2$ for HT424 primer (Phase 1) and Al 2024-T3 adherend (Phase 3).

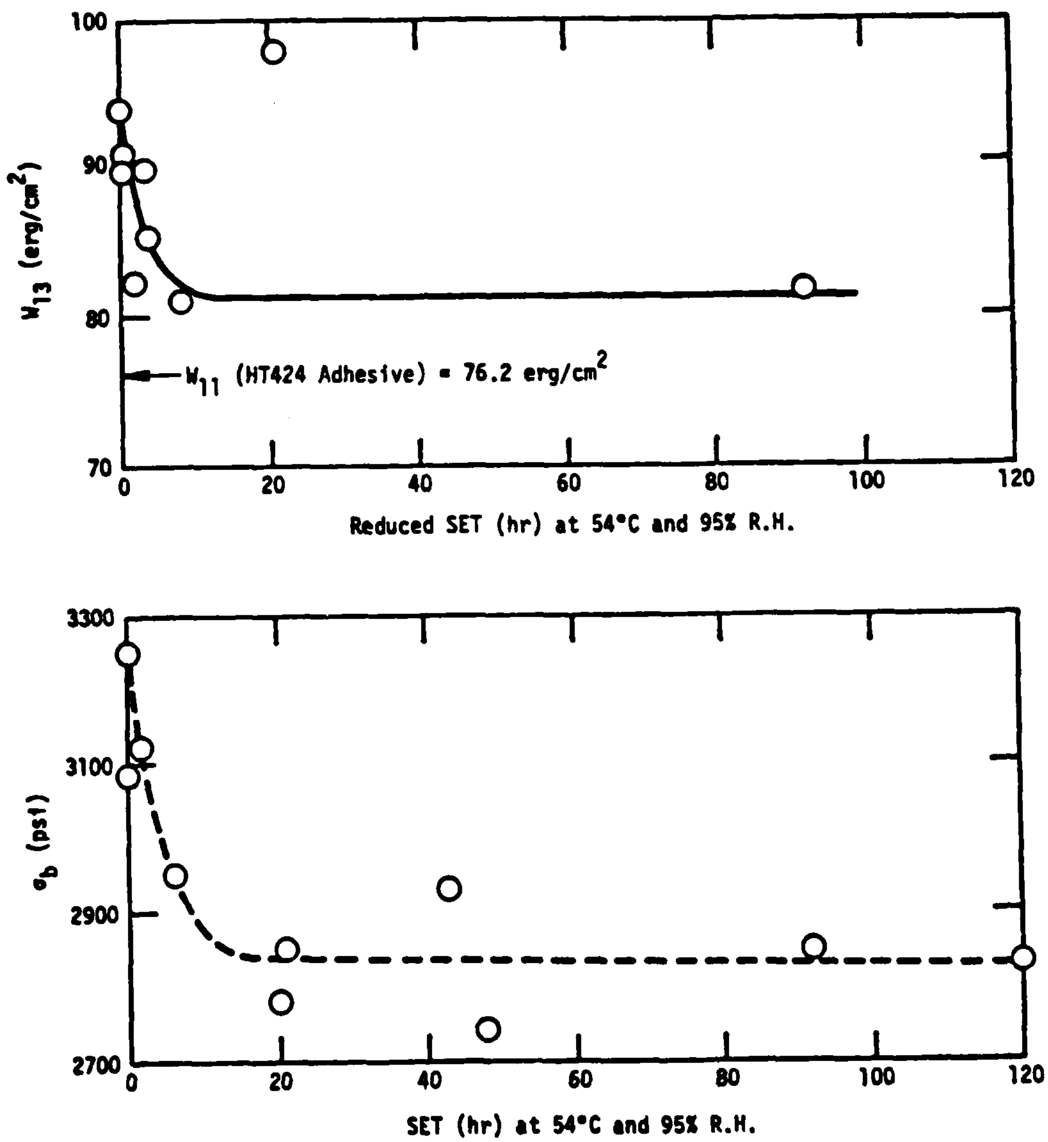


Fig. 1-16 Dependence of interfacial work of adhesion W_{13} (upper curve) and lap shear bond strength σ_b (lower curve) at varied SET.

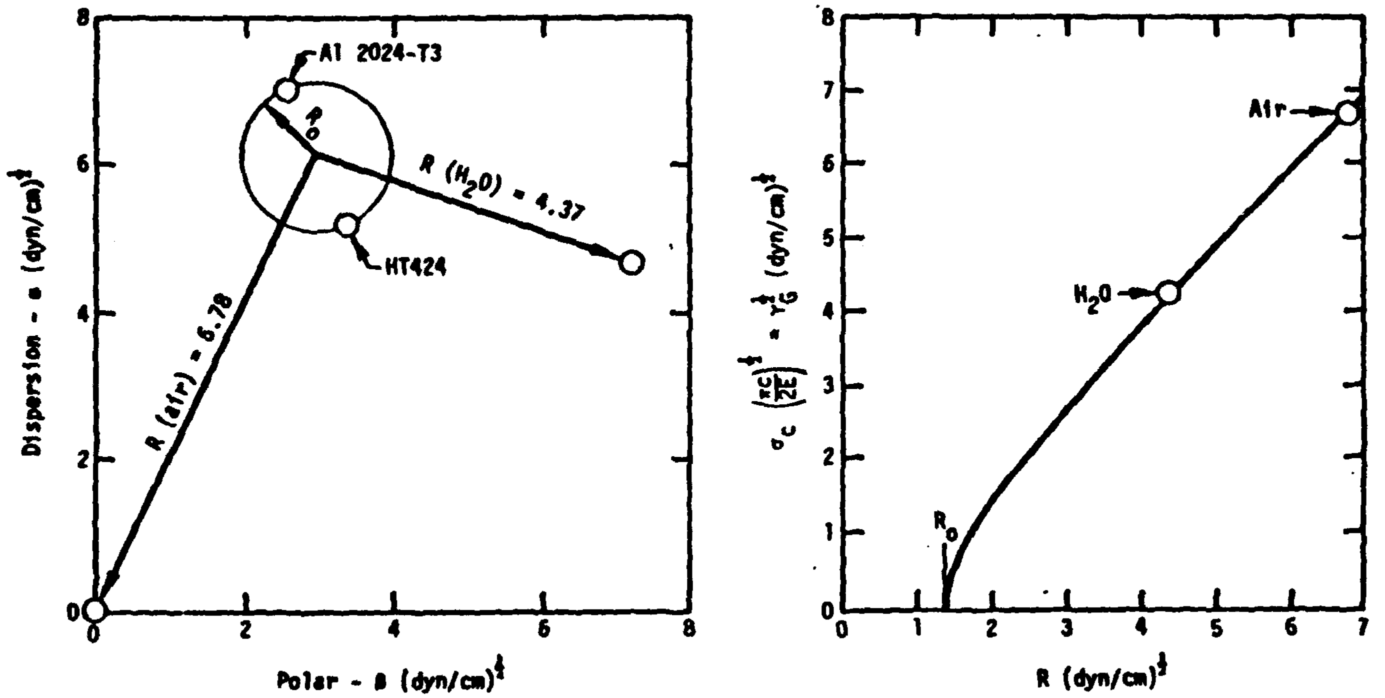


Fig. 1-17 Modified Griffith analysis of the effect of H_2O immersion in reducing the critical interfacial stress σ_I for interfacial failure between HT424 and etched Al 2024-T3 ($\phi_I = 1 - \phi_C = 1.0$).

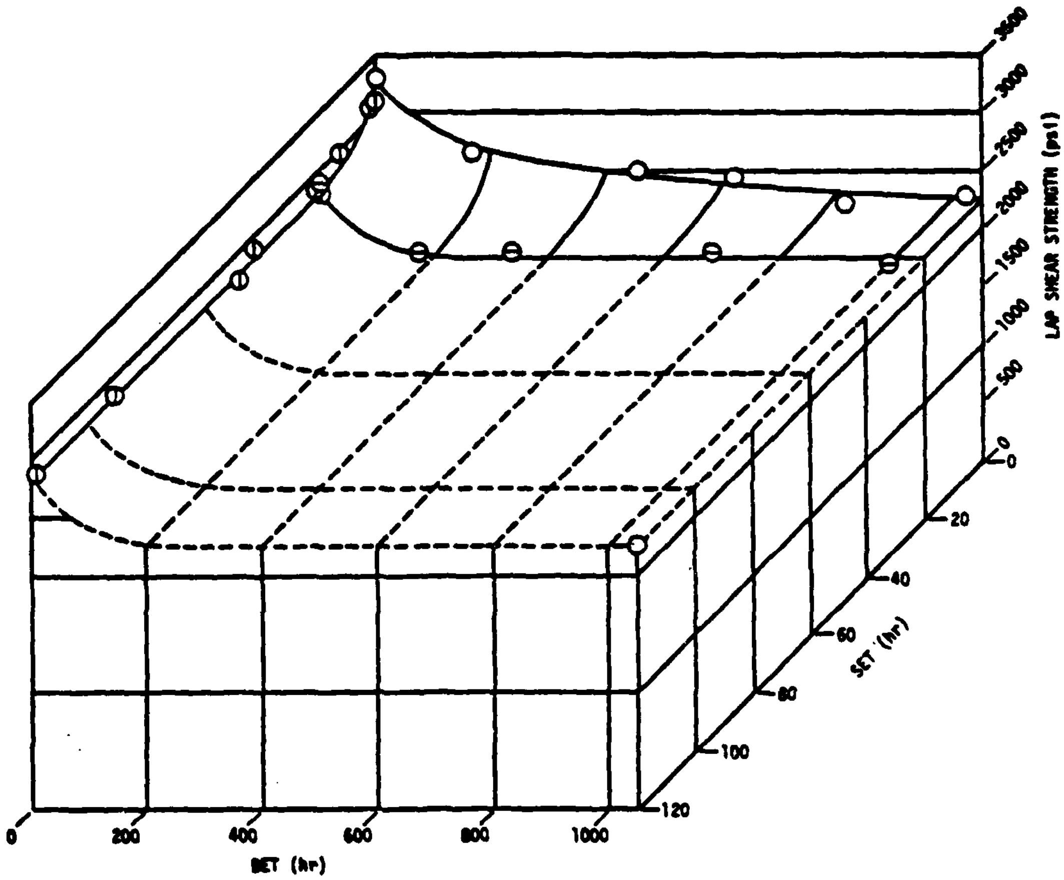


Fig. 1-18 SET and BET response surface for lap shear bond strength for Al 2024-T3 - HT424.

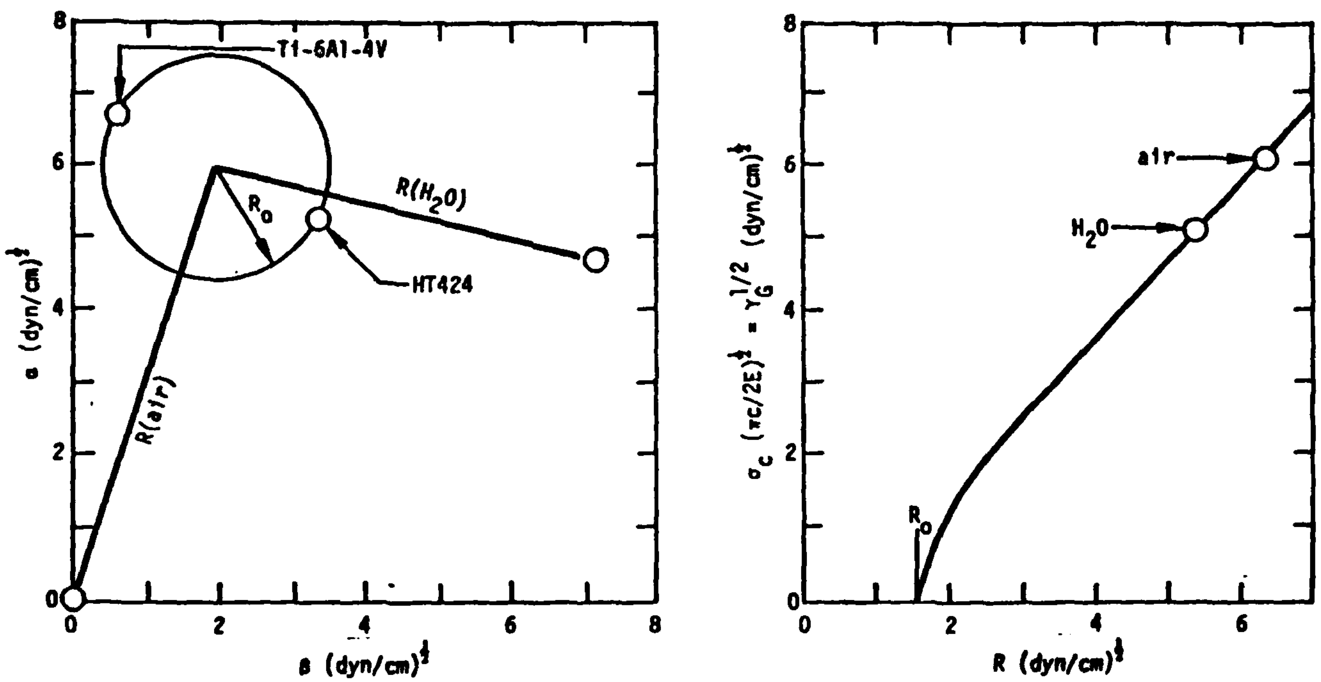


Fig. 1-19 Modified Griffith analysis of the effect of H_2O immersion in reducing critical failure stress σ_I for interfacial failure between HT424 and phosphate-fluoride treated Ti-6Al-4V ($\phi_I = 1 - \phi_C = 1.0$).

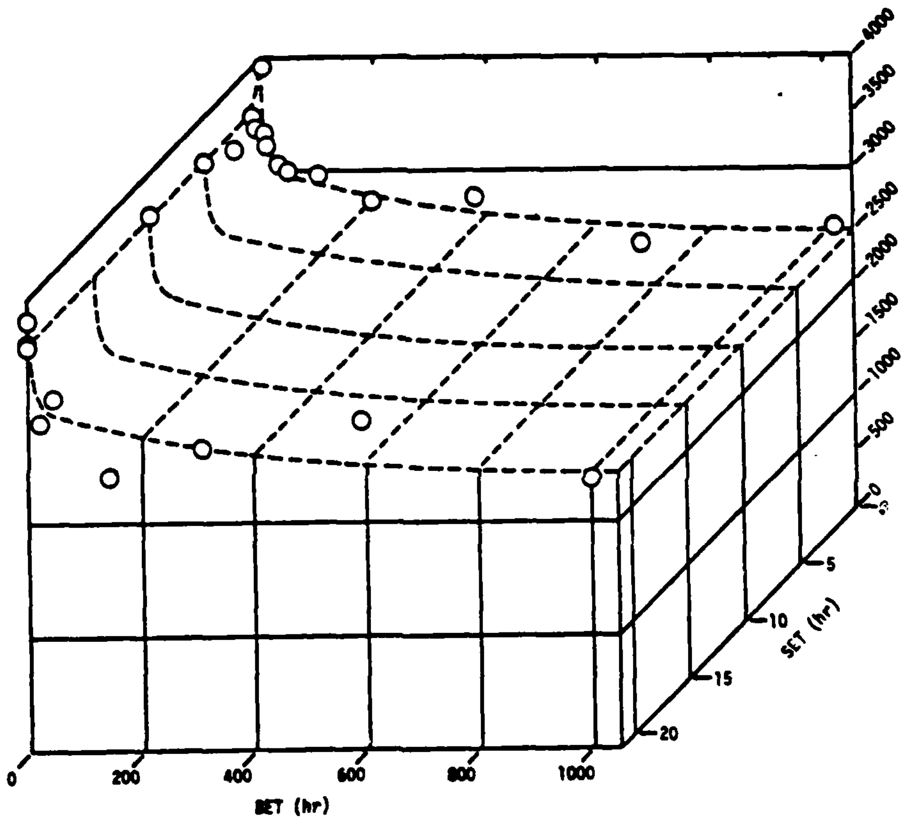
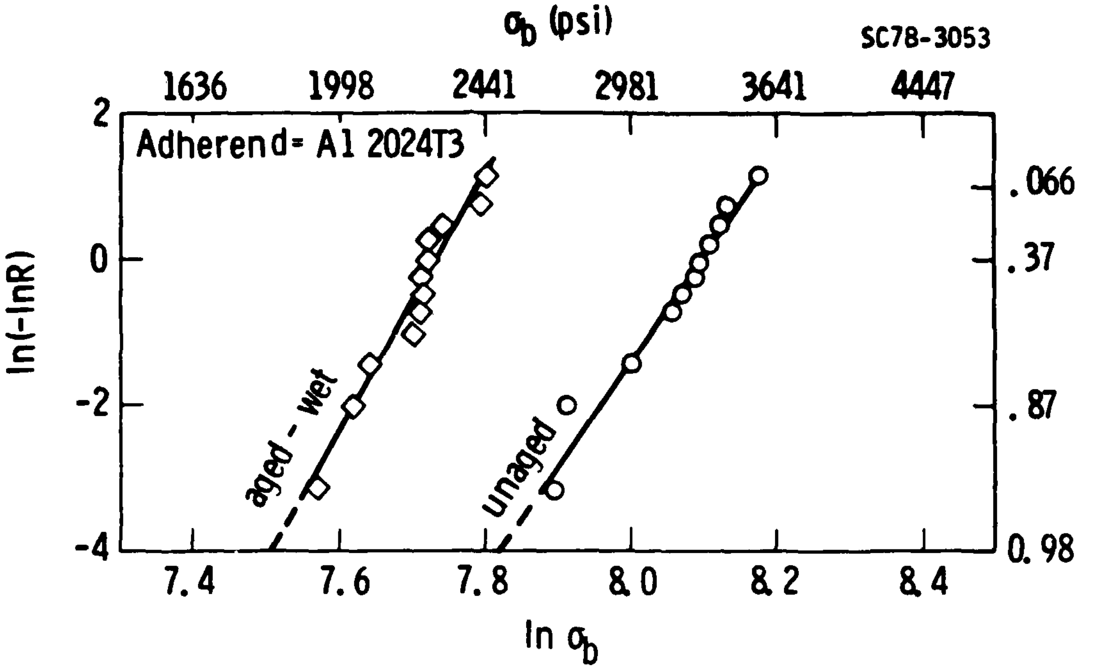


Fig. 1-20 SET vs BET response surface for lap shear bond strength for Ti-6Al-4V - HT424.



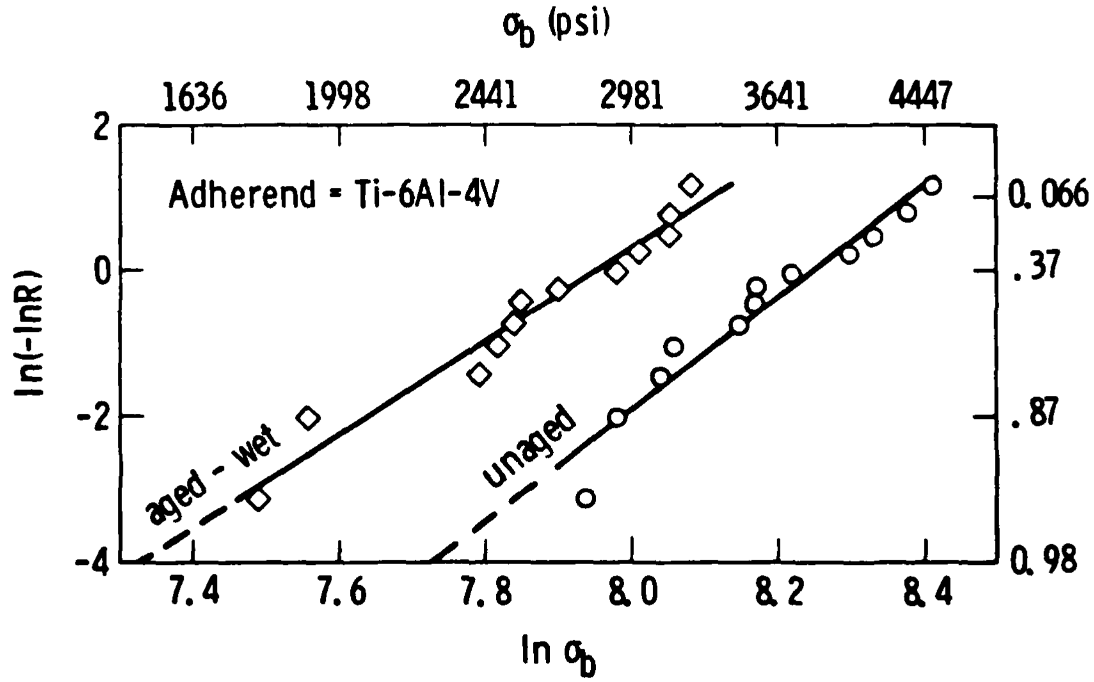


Fig. 1-21 Comparison of Weibull shear strength distributions for aluminum (upper view) and titanium (lower view) adherends.

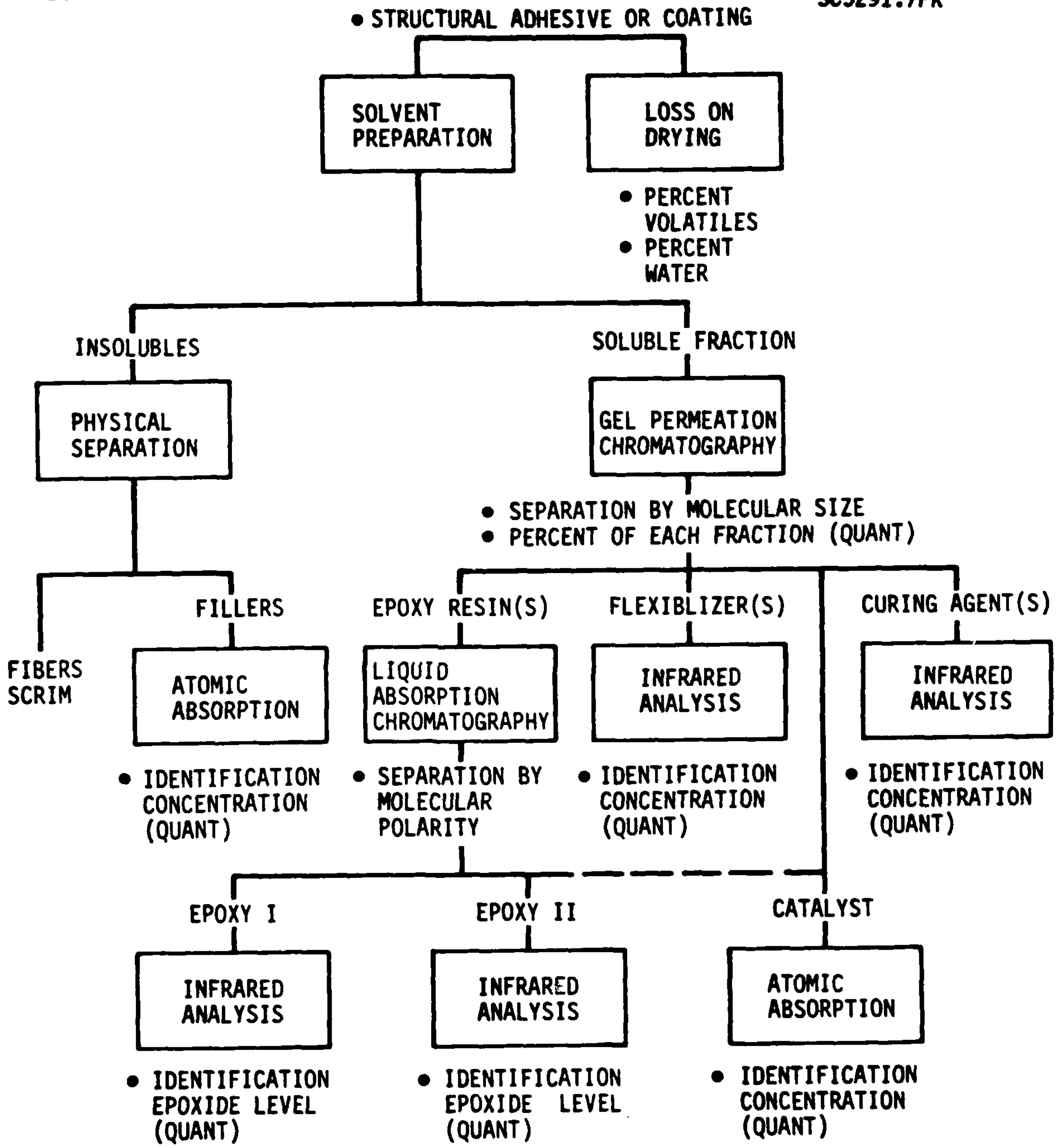


Fig. 1-22 Chemical analysis flow chart.

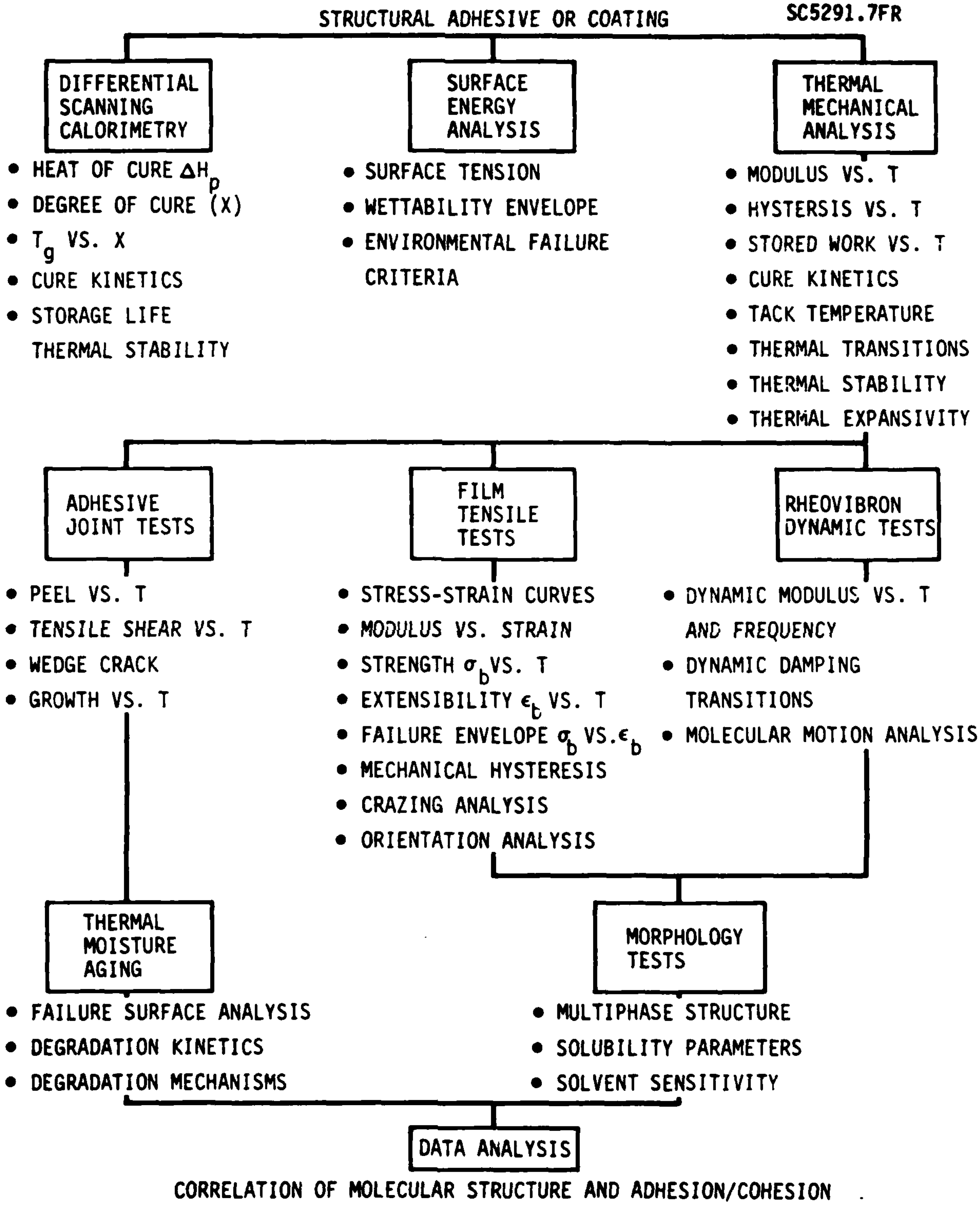


Fig. 1-23 Physical and mechanical analysis flow chart.

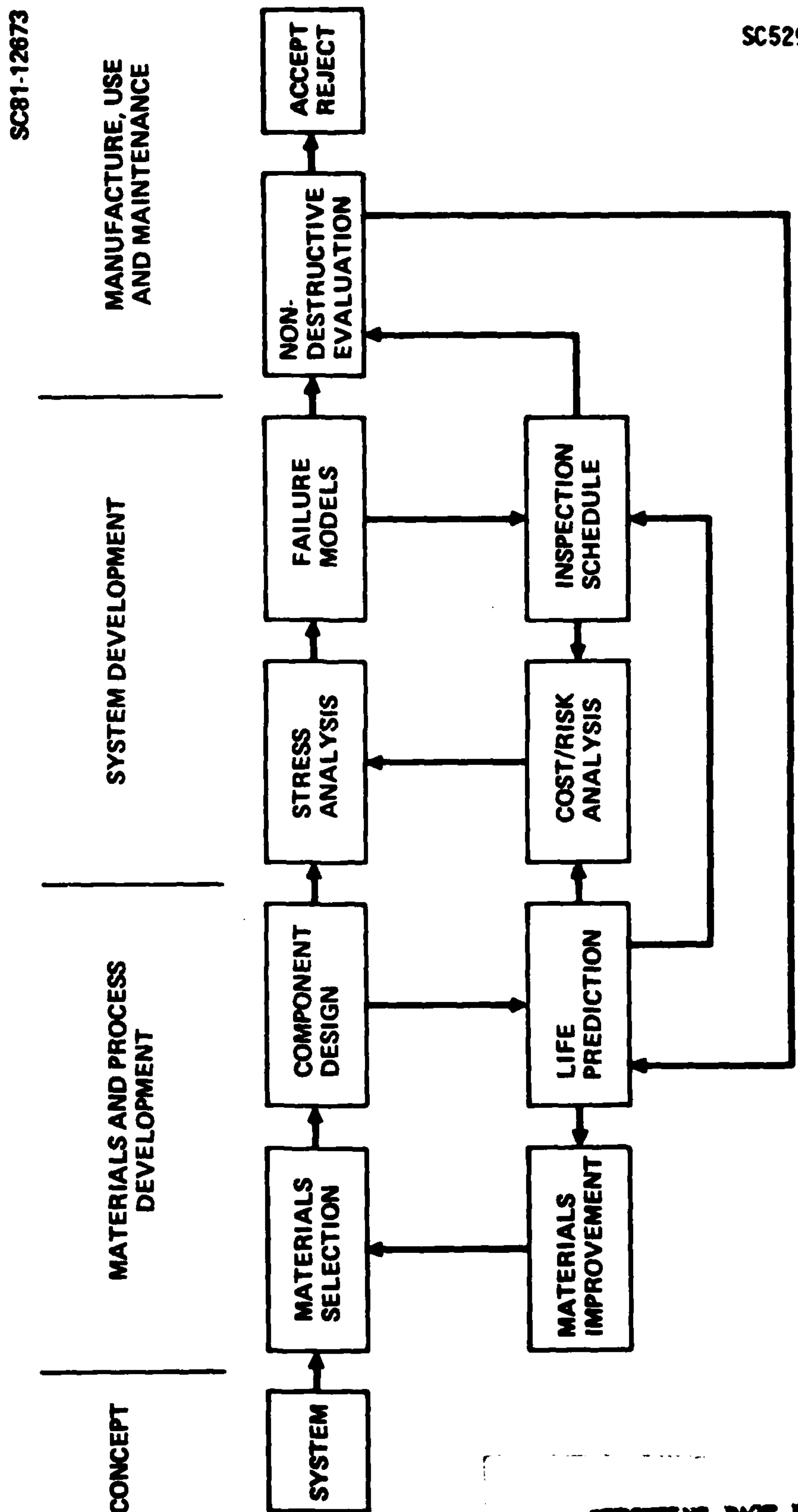


Fig. 2-1 Logic flow chart for predictive design methodology.

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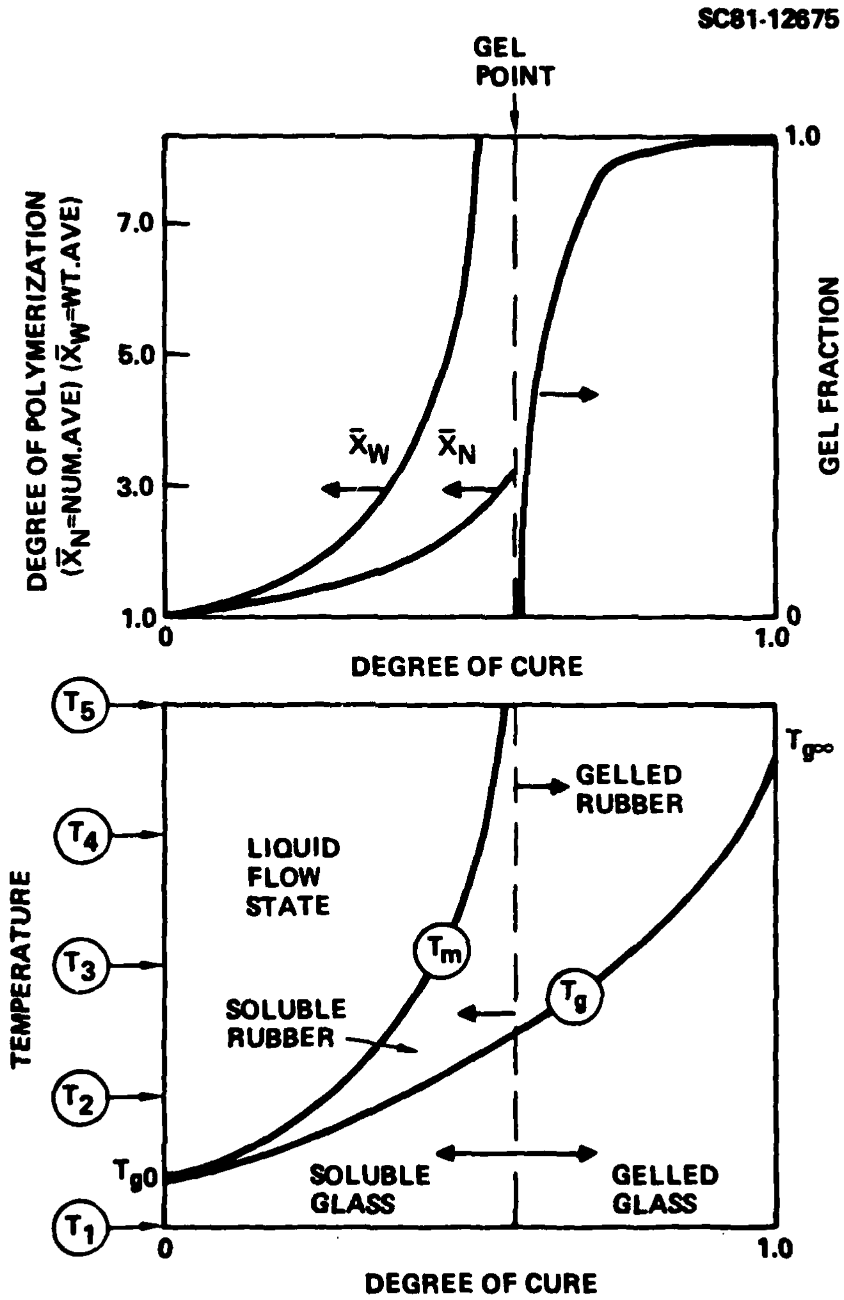

Fig. 2-2 (Upper): Change in molecular weight distribution and sol-gel state with degree of cure (idealized).
(Lower): The effect of degree upon glass transition temperature T_g and melt temperature T_m for liquid flow (idealized).

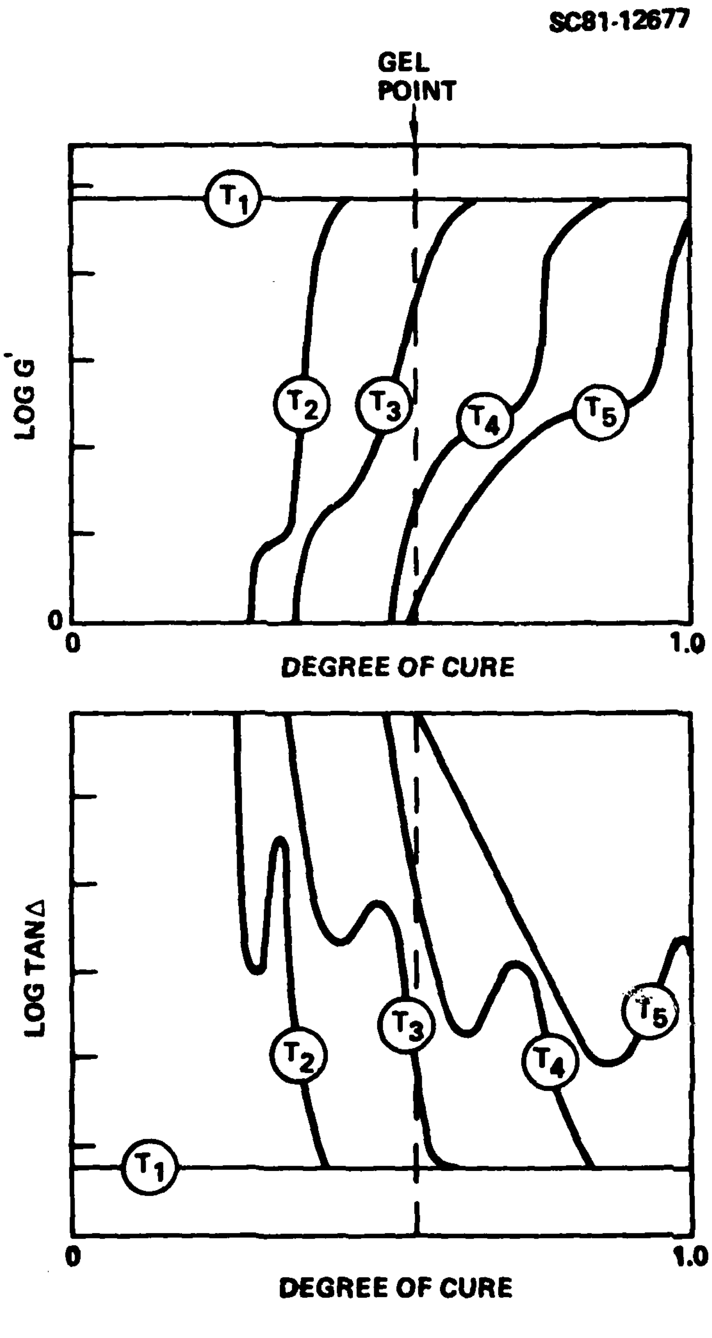

Fig. 2-3 Idealized isothermal dynamic mechanical monitoring of degree of cure in terms of shear storage modulus G' (upper view) and loss tangent tan δ (lower view).

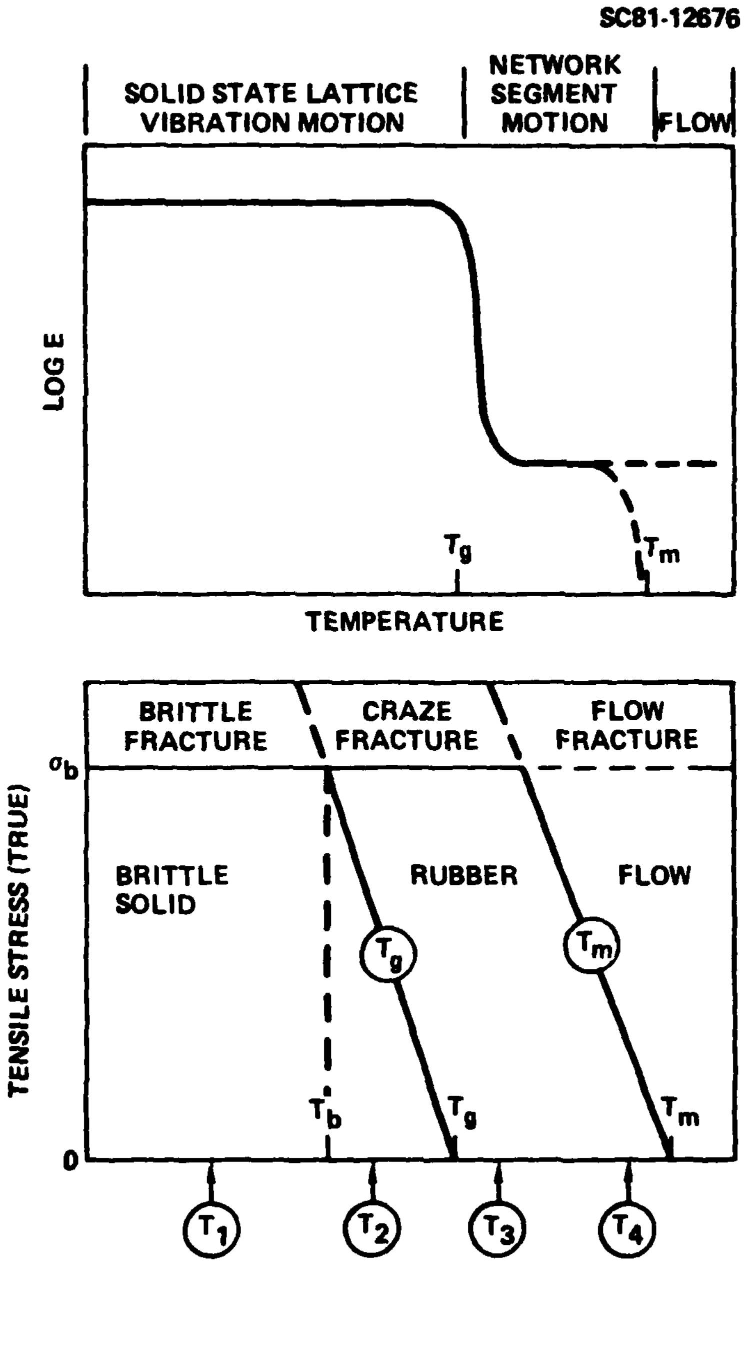

Fig. 2-4 Thermal scanning of fully cured matrix for tensile modulus (upper view) and stress-temperature response (lower view) at constant time of loading (idealized).

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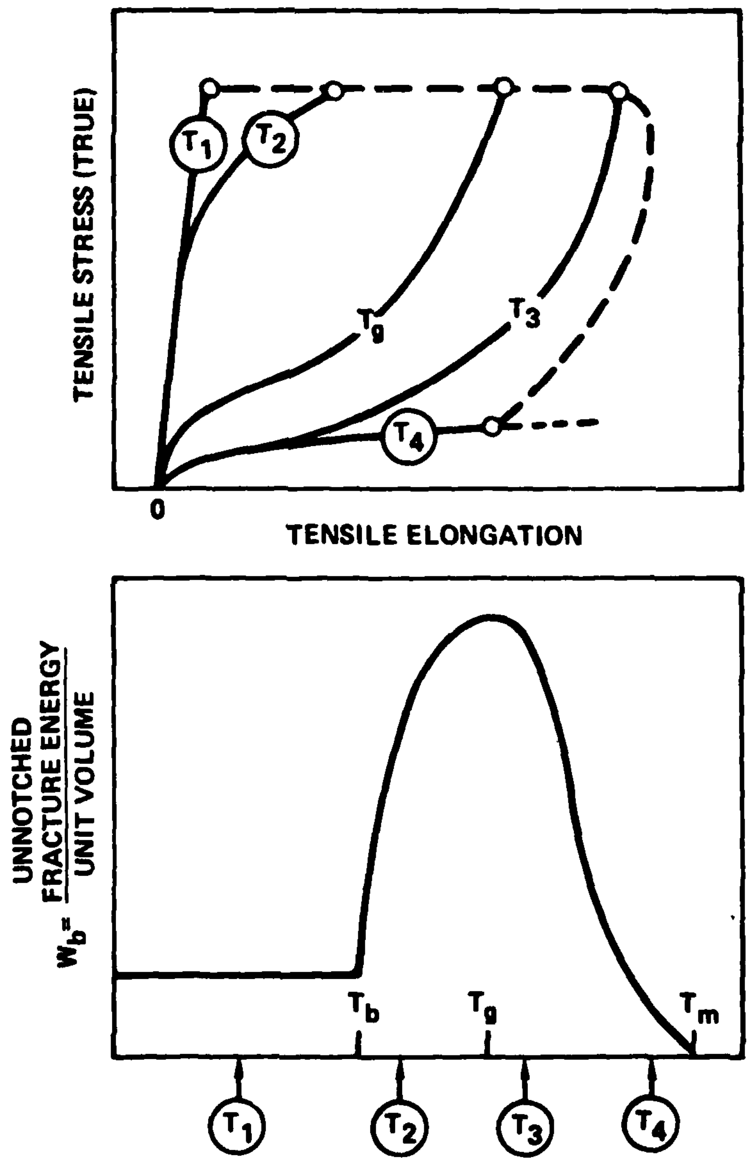

Fig. 2-5 Characteristic tensile stress-strain and fracture response (upper view) and temperature profile of unnotched tensile fracture energy (lower view).

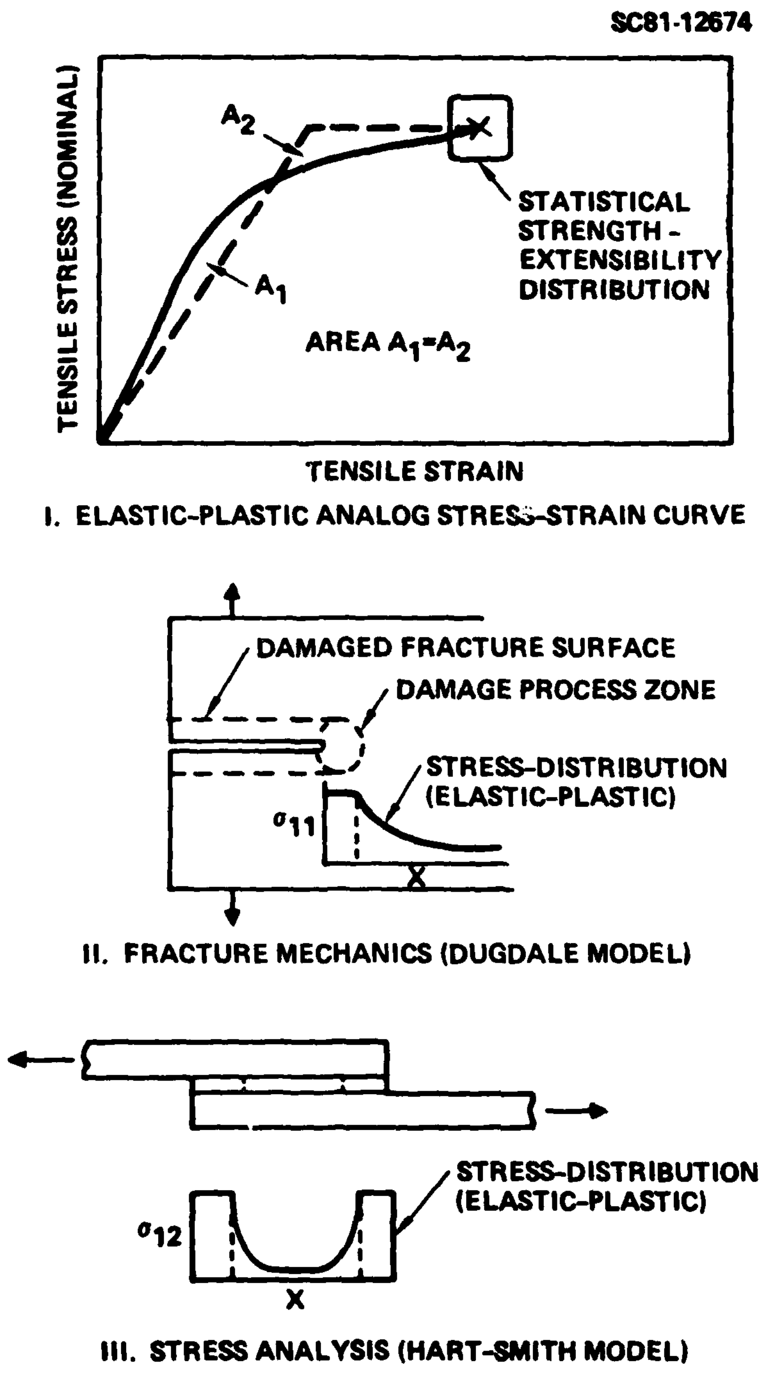

Fig. 2-6 Conversion of measured stress-strain to elastic-plastic analog (I) and introduction into fracture mechanics (II) and stress analysis (III) predictive models.

SC81-13600

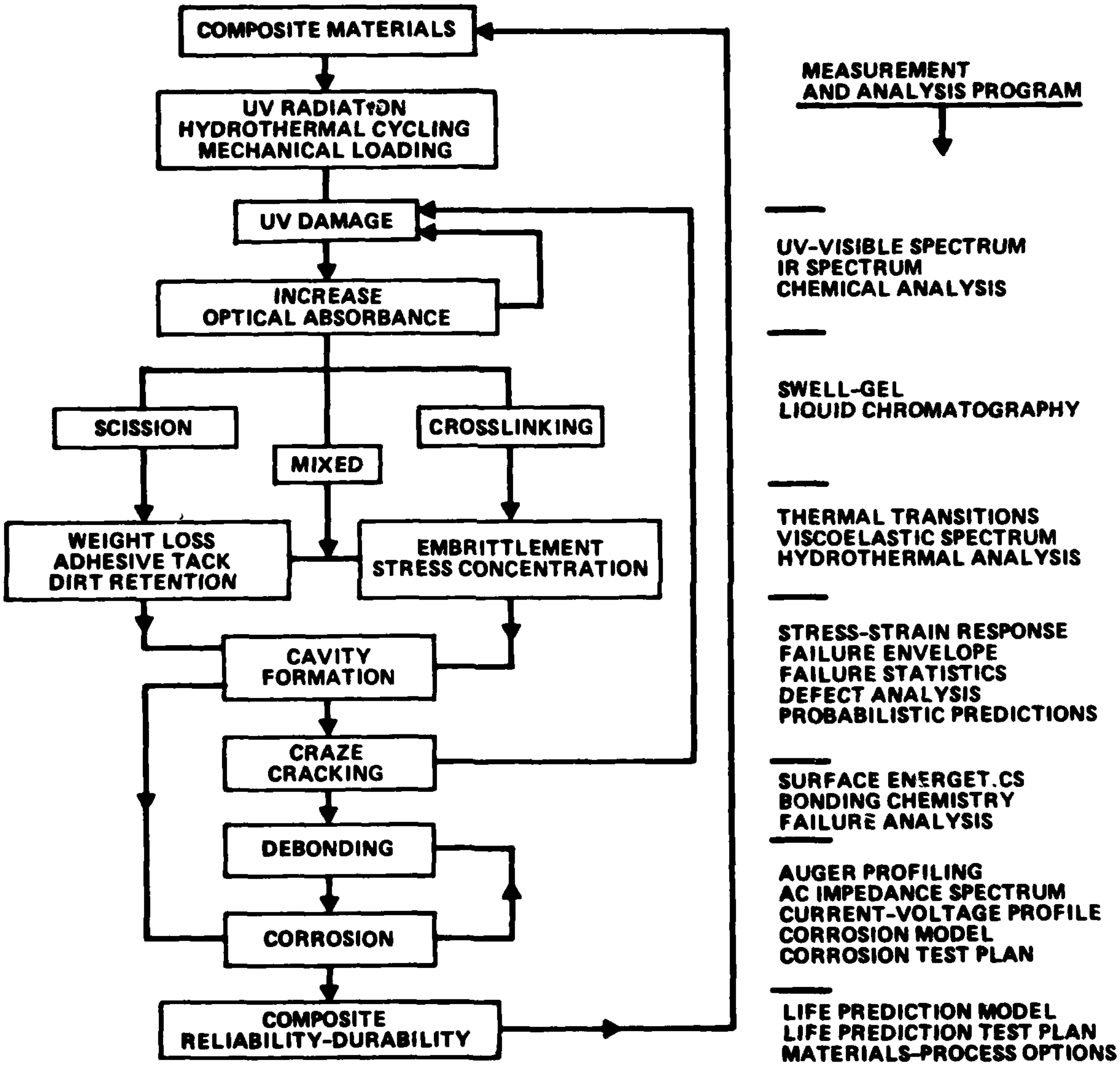

Fig. 2-7 General laminate life prediction program.

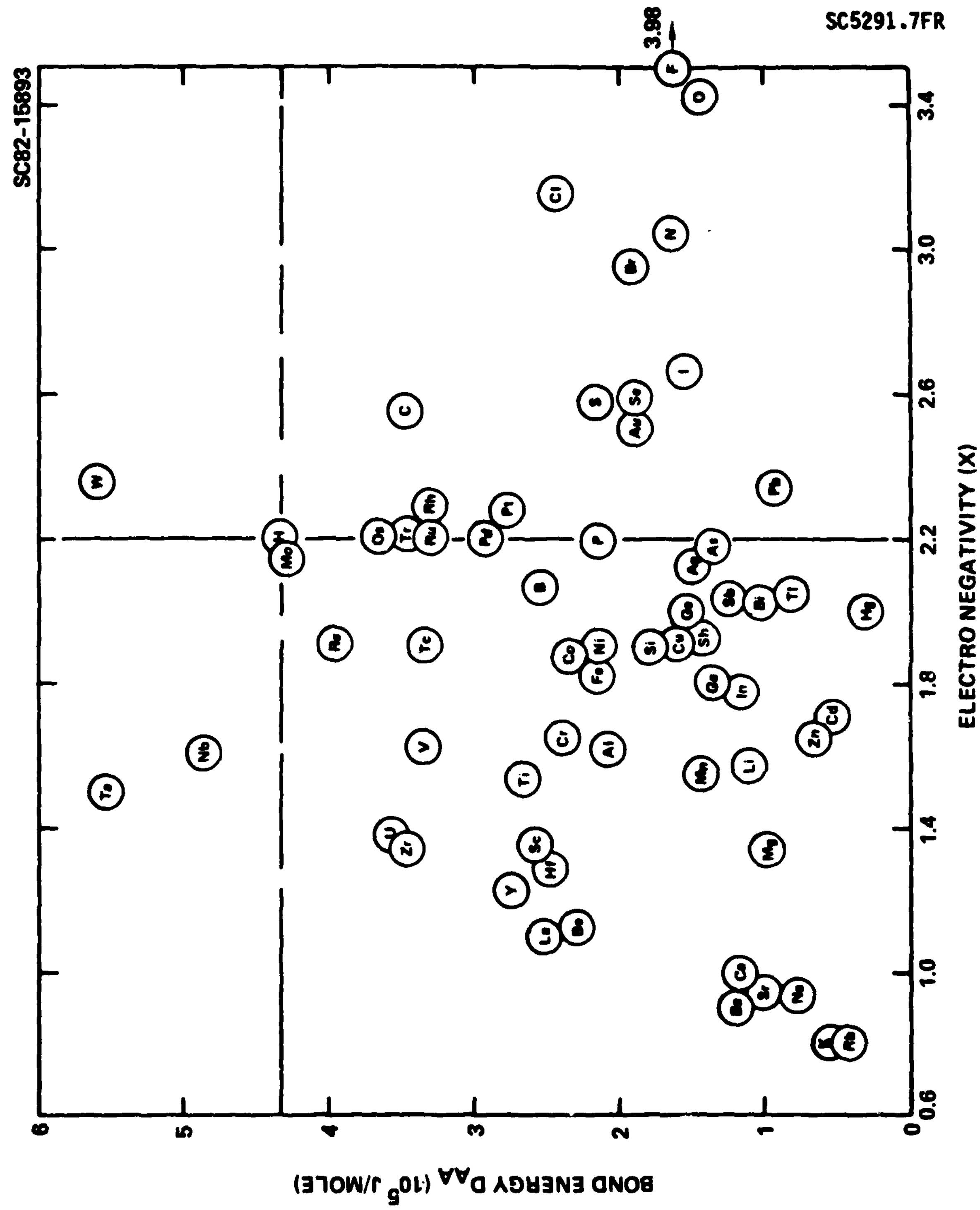

Fig. 3-1 Covalent bond energy D_{AA} and electronegativity X for the elements.

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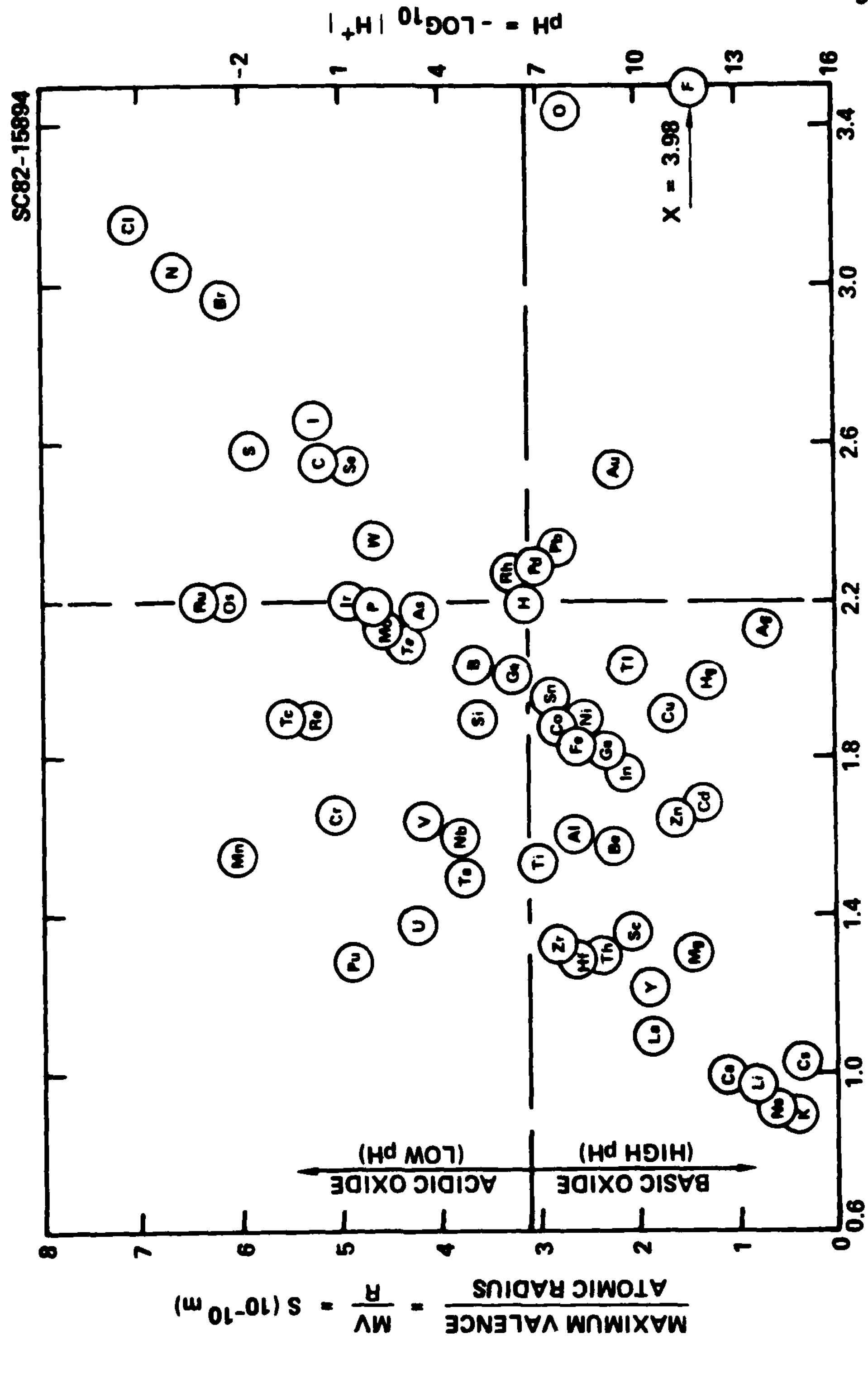


Fig. 3-2 The maximum valence to atomic radius ratio, MV/R vs electronegativity.

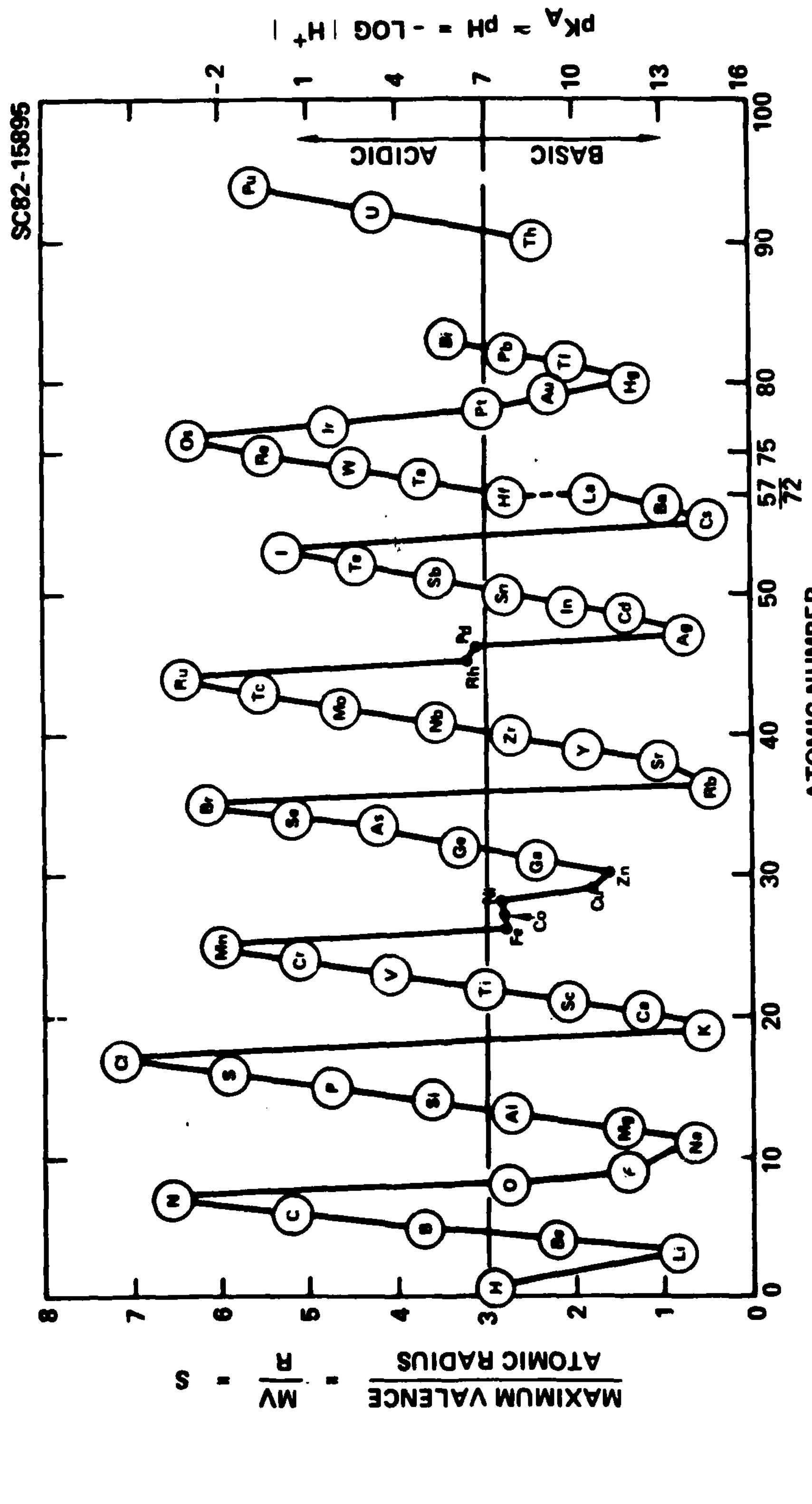


Fig. 3-3 Acidity index pH = 16 - 3S vs atomic number.

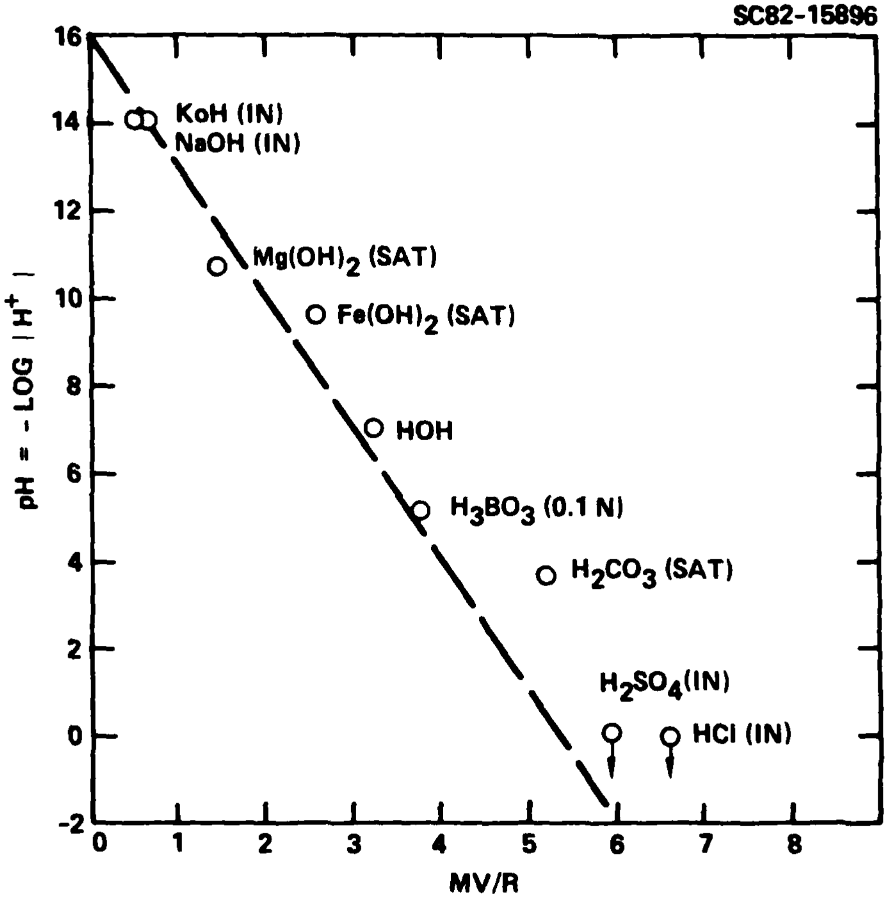


Fig. 3-4 pH vs (MV/R) for acids and bases.

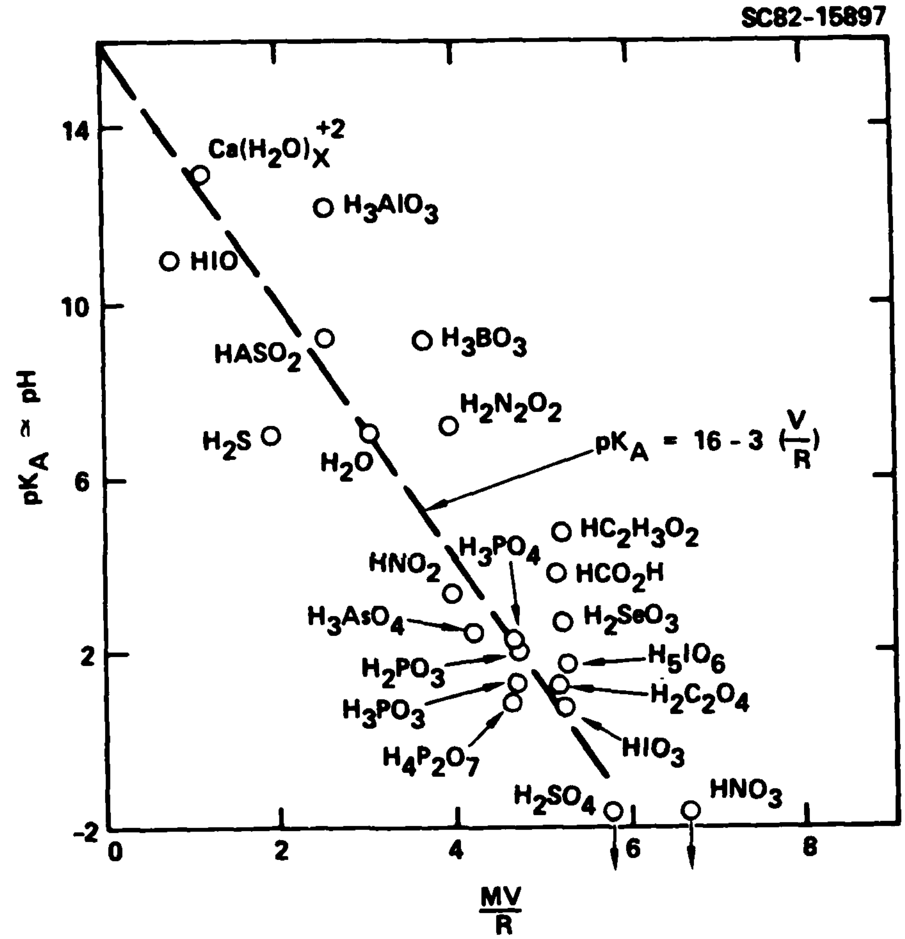


Fig. 3-5 Acid dissociation index pK_A vs (V/R) for miscellaneous acids and bases at varied valence.

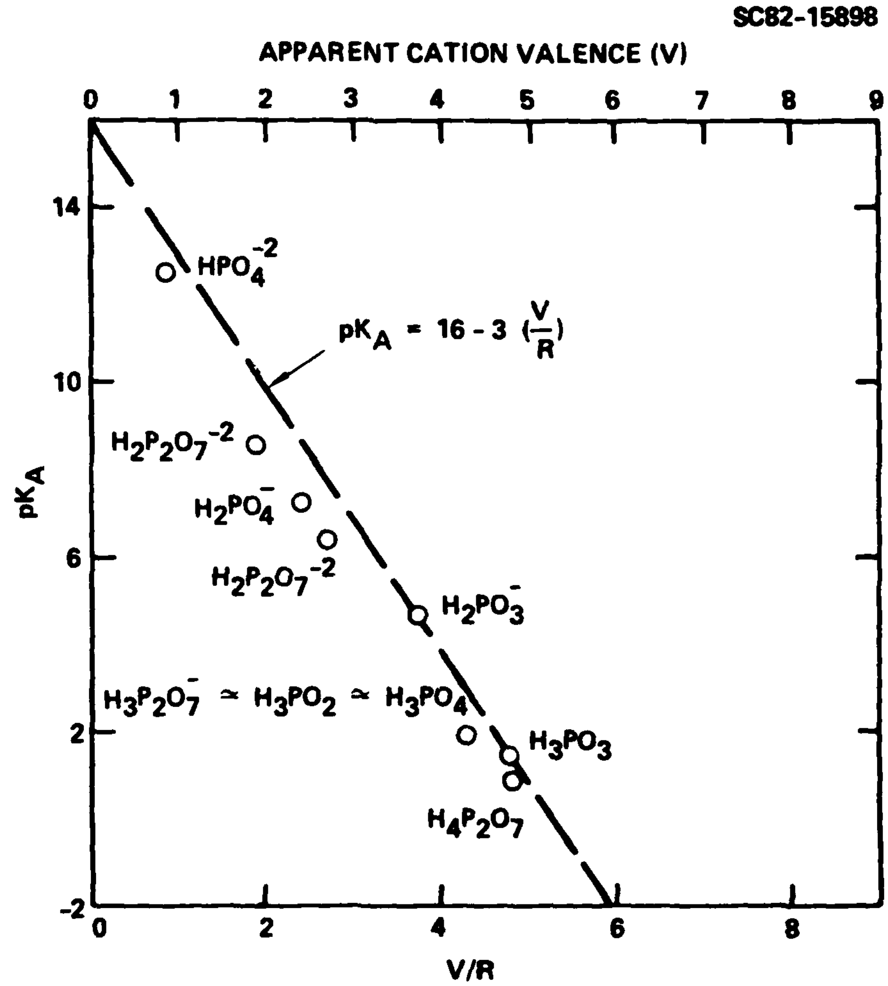


Fig. 3-6 Acid dissociation index pK_A vs apparent cation valence V and V/R.

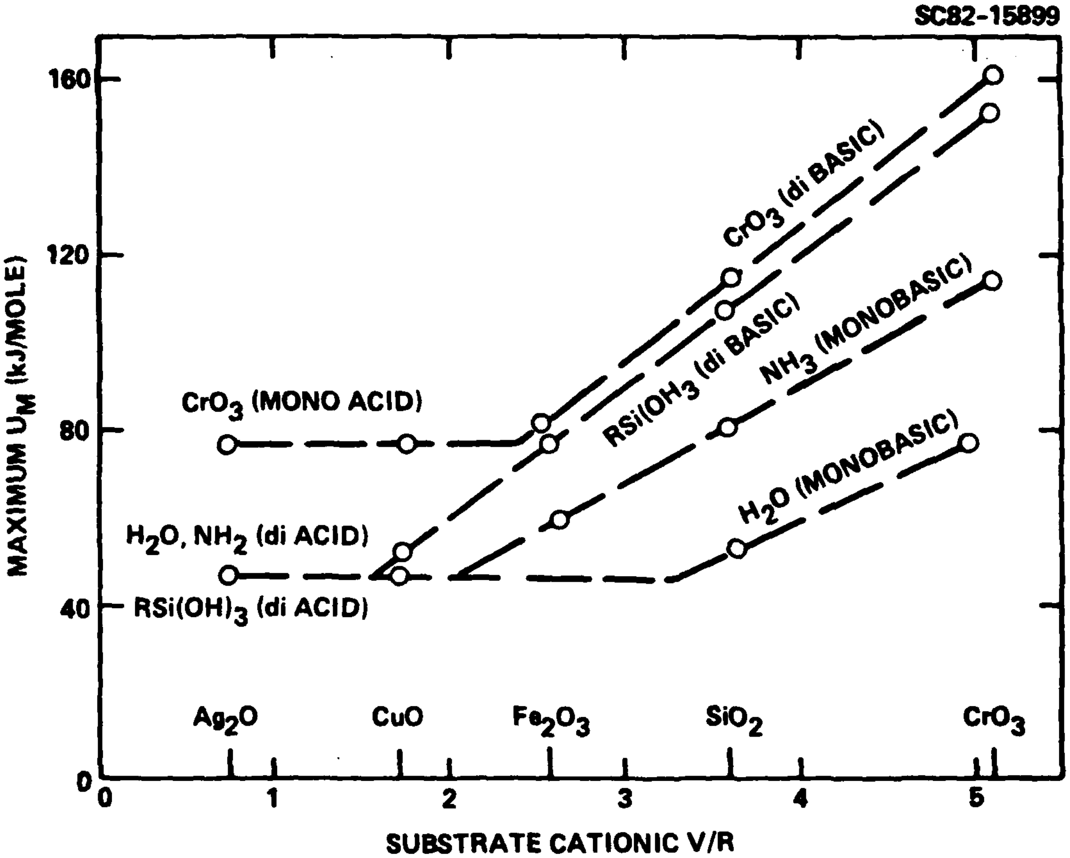


Fig. 3-7 Calculated maximum Coulomb energy U_m between adsorbate and substrate oxides.

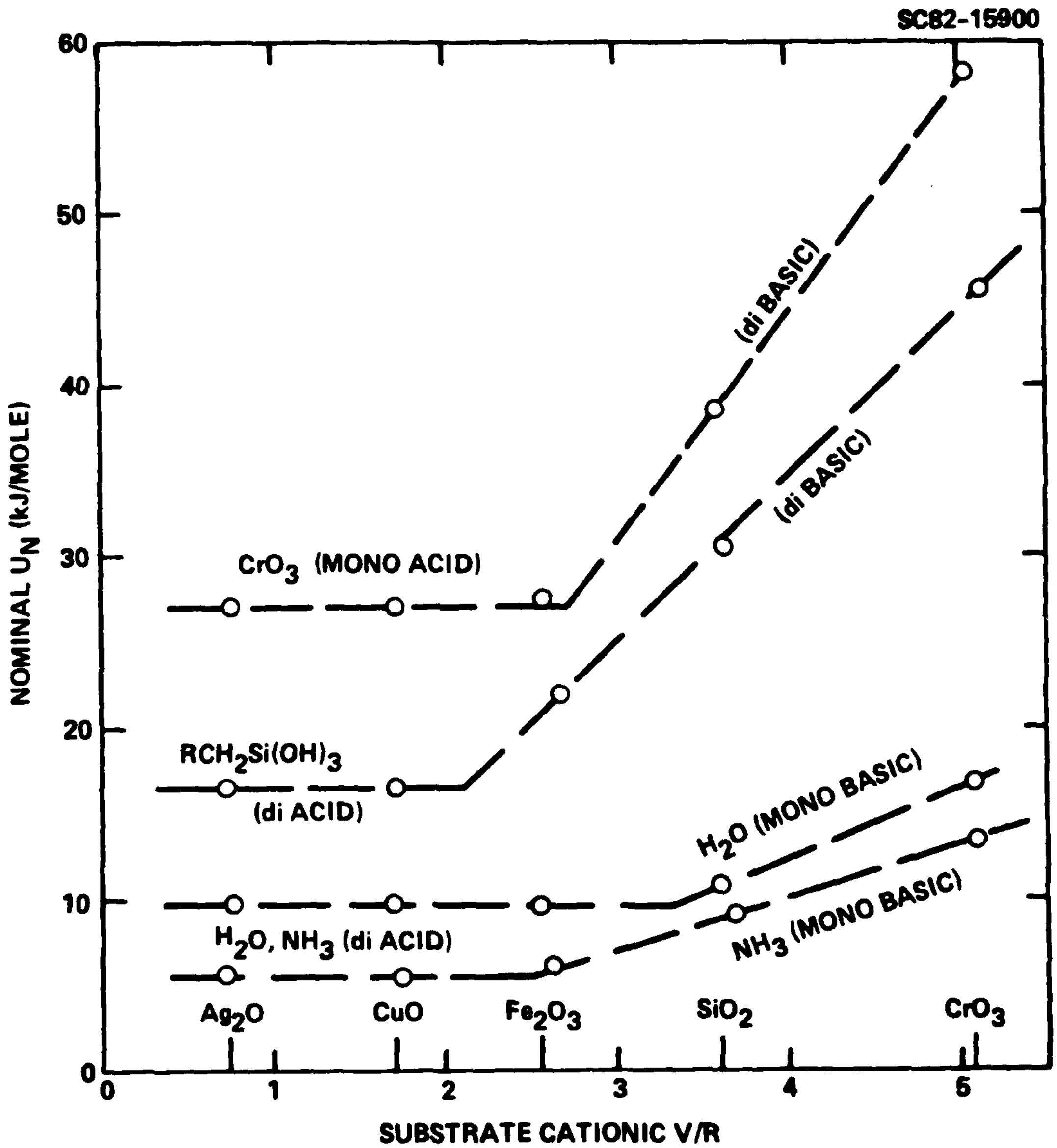


Fig. 3-8 Calculated nominal Coulomb energy U_N between absorbate and substrate oxides.

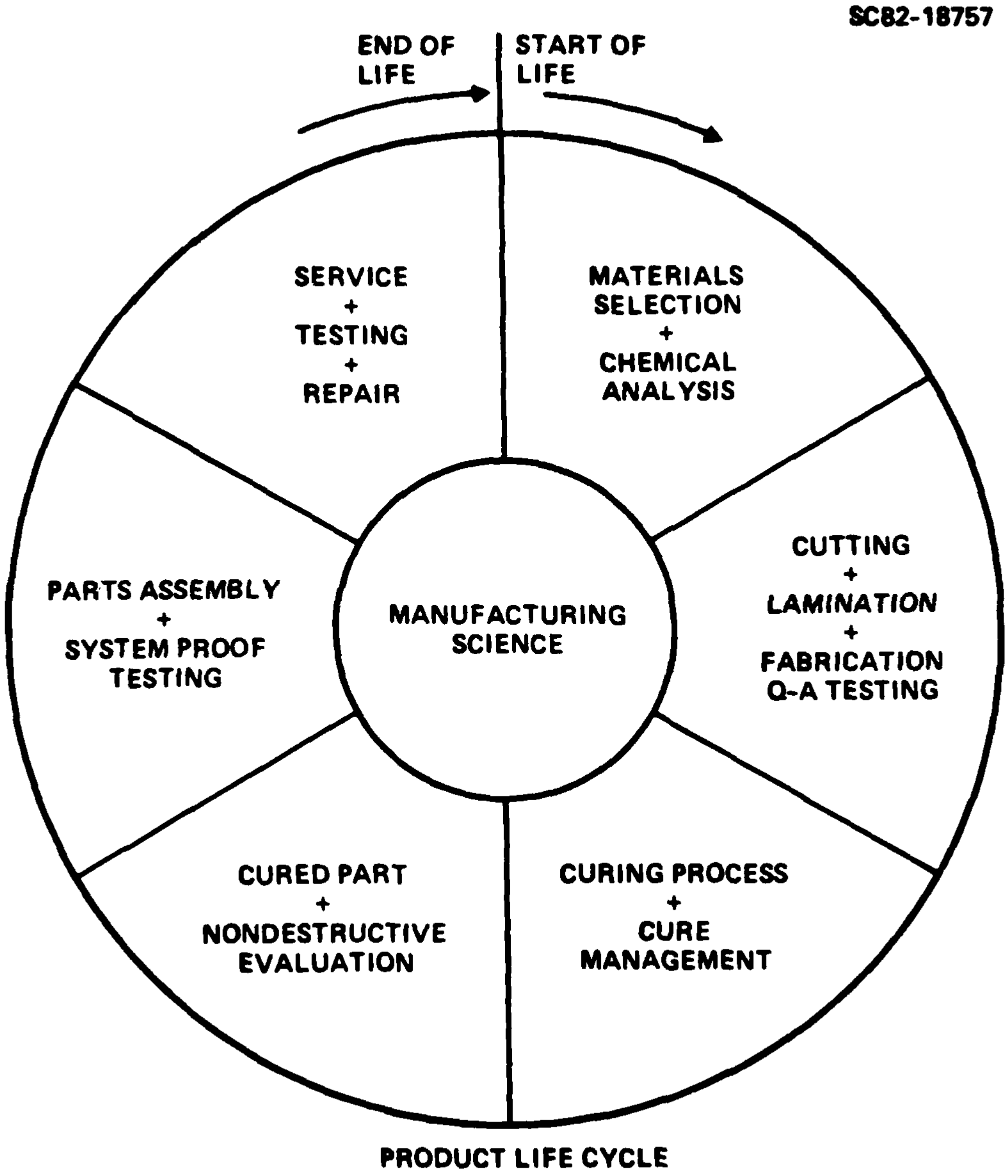


Fig. 4-1 Central role of manufacturing science in the product life cycle.

SC82-16509

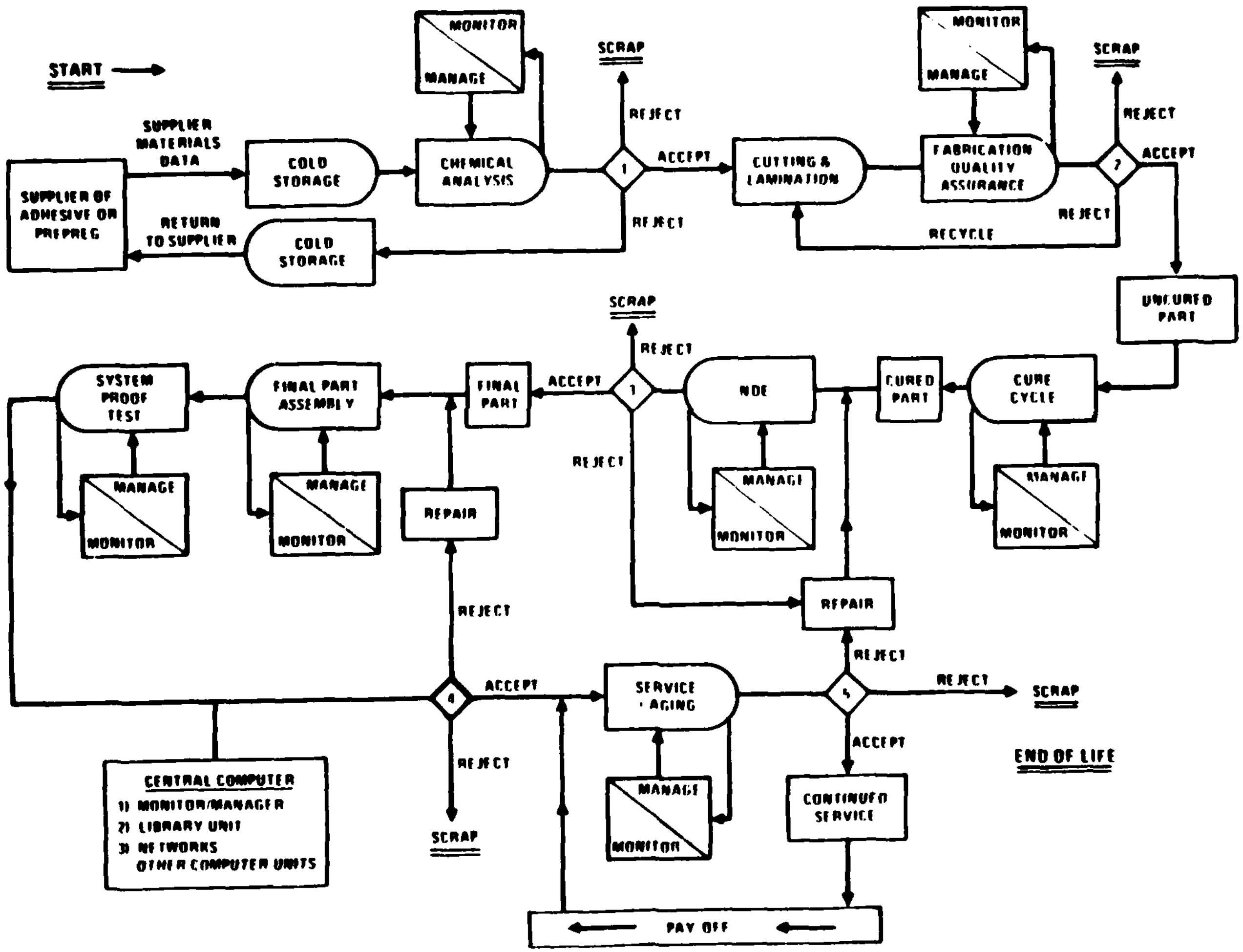


Fig. 4-2 Illustrative computer aided manufacture-service-repair cycle.

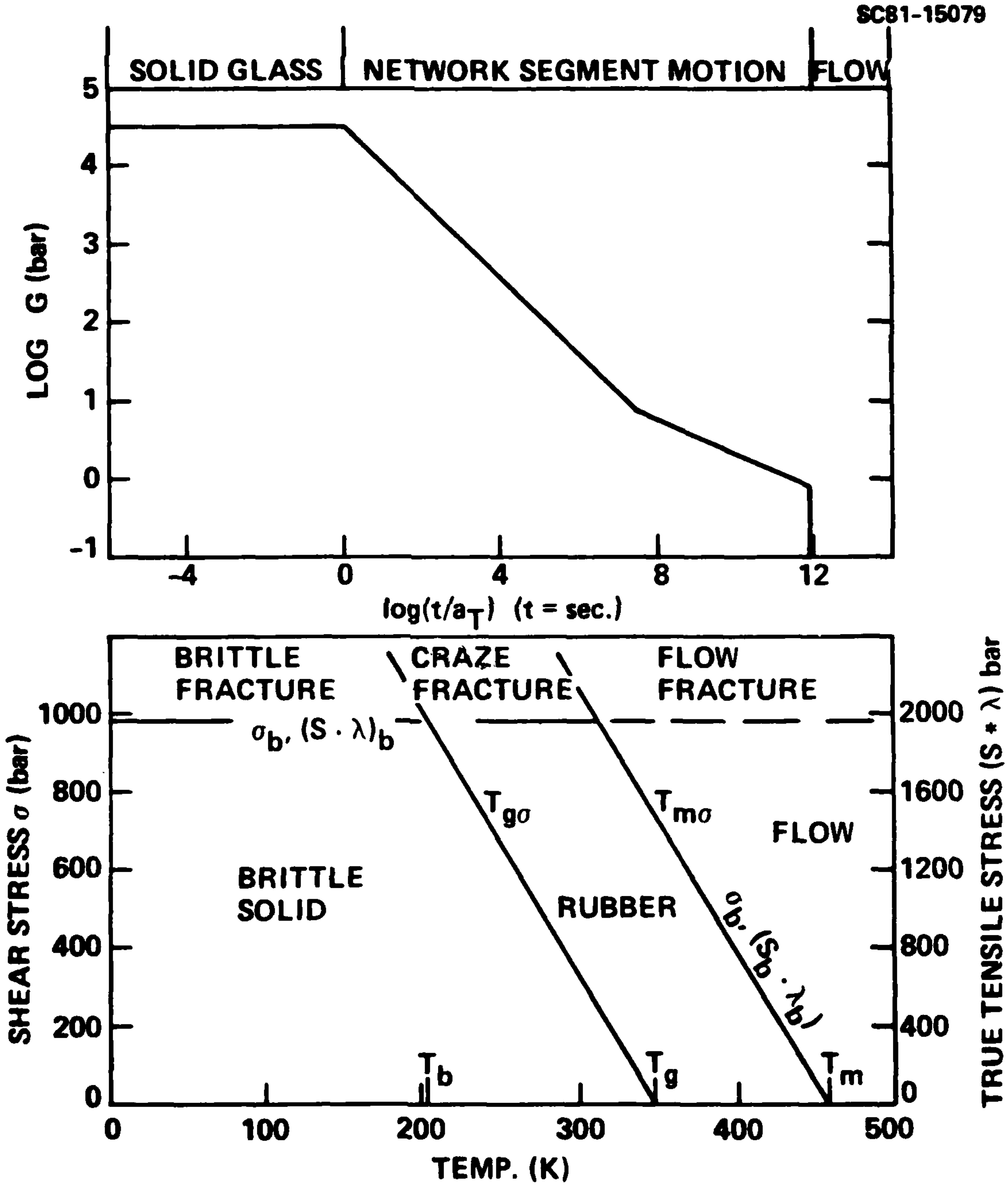
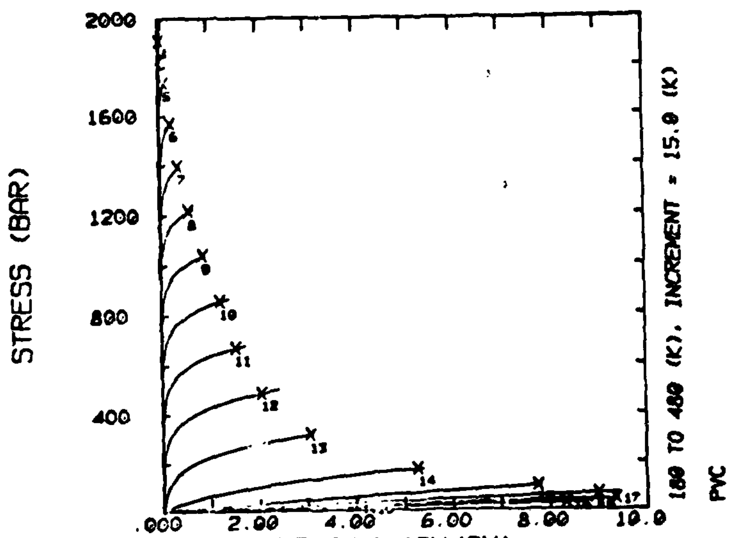
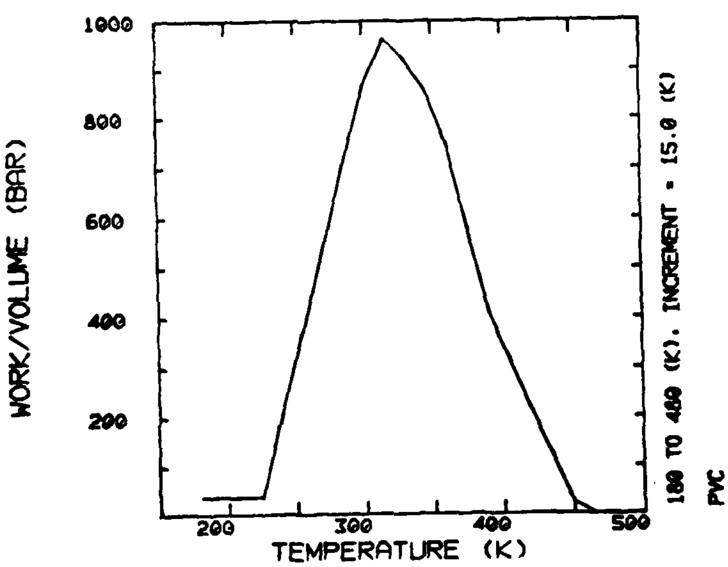


Fig. 4-3 Calculated shear modulus G vs reduced relaxation time t/a_T (upper curve) and stress-temperature functions for yield and fracture (lower curves).



STRESS VS STRAIN - TENSILE - FIXED T=1.00 SEC



WORK VS TEMP - TENSILE - FIXED T=1.00 SEC

Fig. 4-4 Computed estimates of nominal tensile stress vs strain response and failure (indicated by X in upper curves) and fracture energy (lower curve) of linear polyvinyl chloride (T_g = 348 K, M_n = 8.53E5 gm/mole).

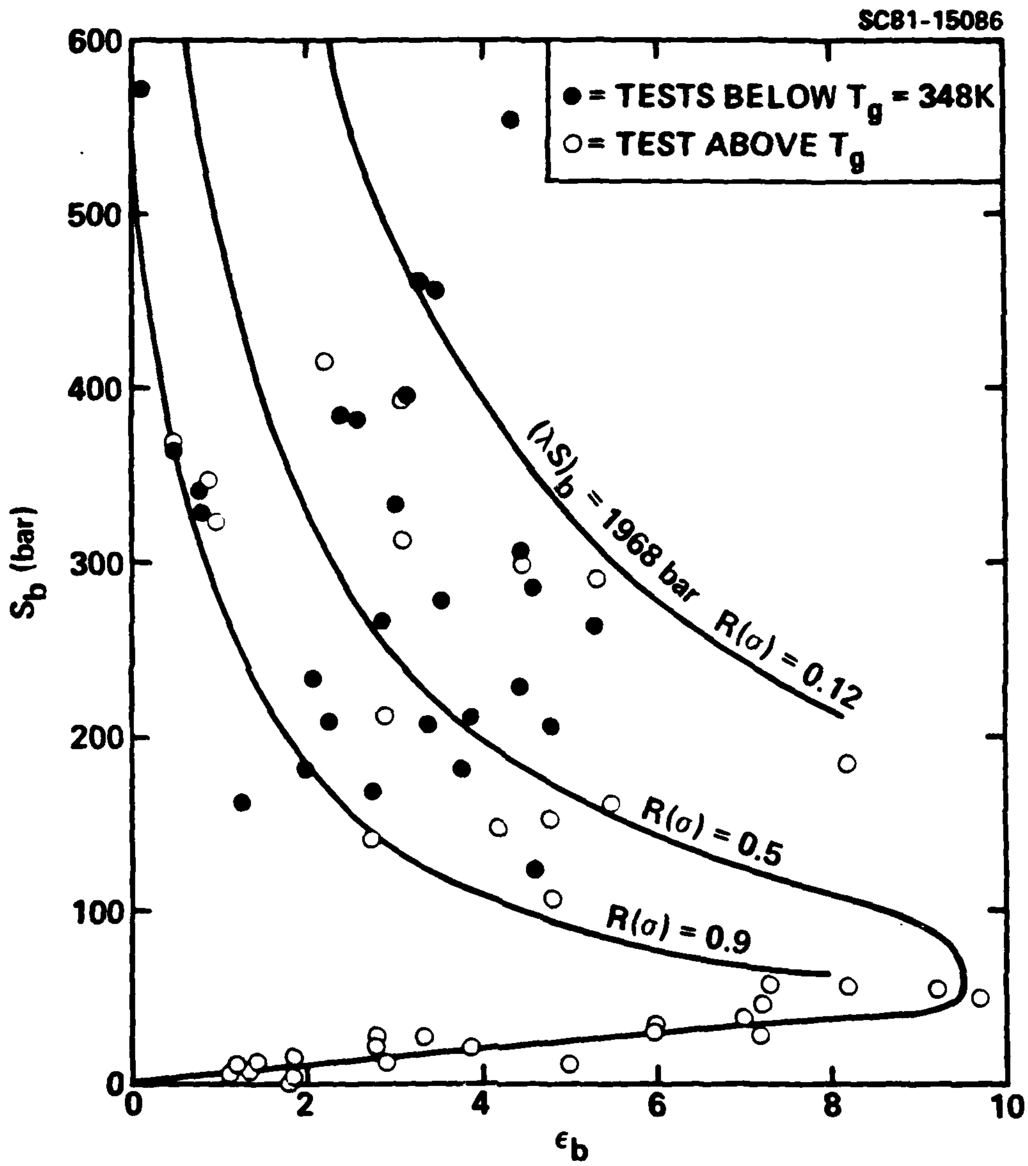


Fig. 4-5 Experimental values of nominal tensile stress S_b vs extensibility ϵ_b for polyvinyl chloride film (T_g = 346 K, M_w = 1.16E6 gm/mole).

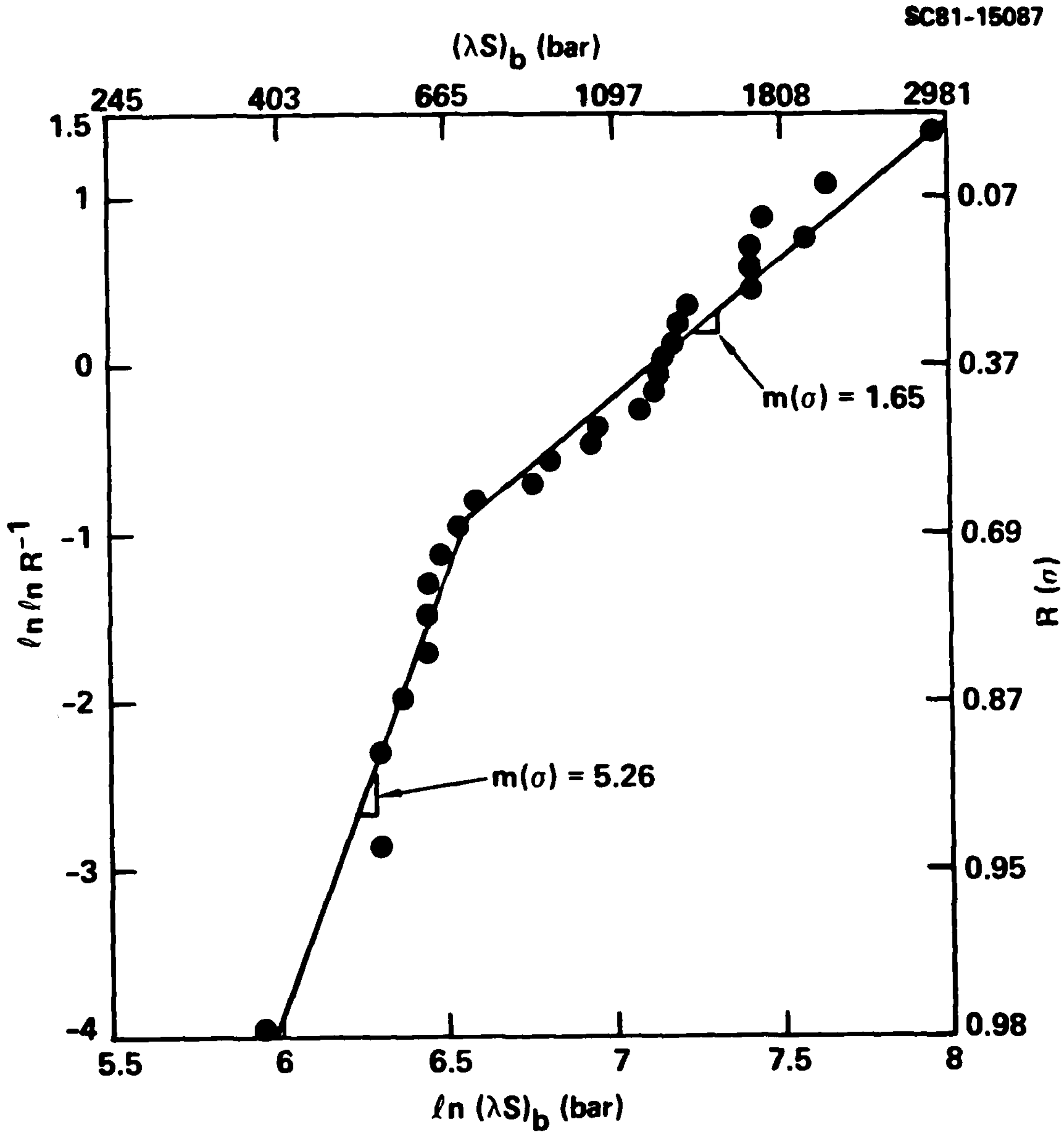


Fig. 4-6 Experimental reliability distribution $R(\sigma)$ for true tensile strength $(\lambda S)_b$ of polyvinyl chloride below T_g.

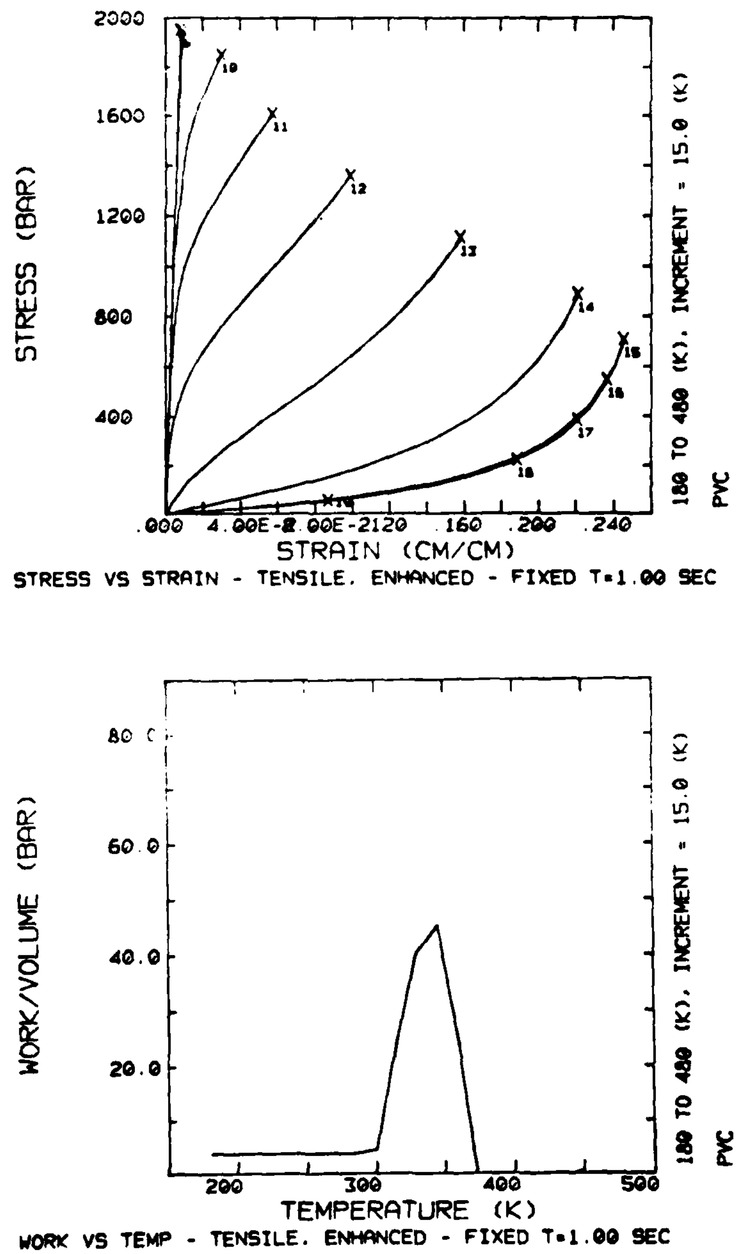


Fig. 4-7 Computed estimates of nominal tensile stress vs strain response (upper curves) and fracture energy (lower curve) for crosslinked PVC.

SC81-15146

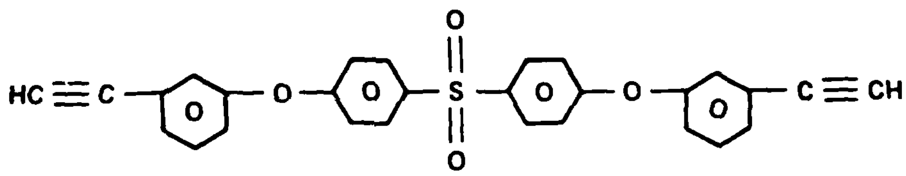
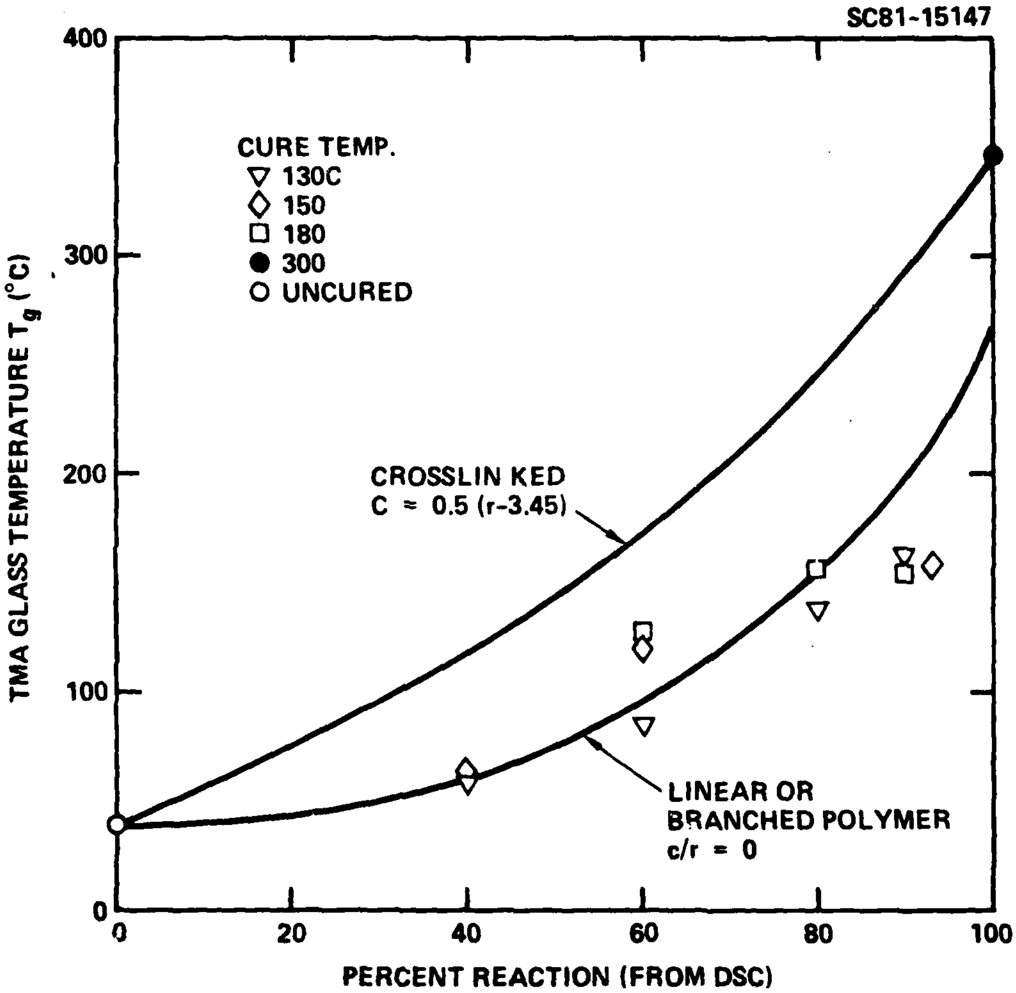


Fig. 4-8 Model ATS oligomer structure.



Fi~ 4-9 Experimental and theoretical (solid curves) values of T_g for ATS as a function of cure path.

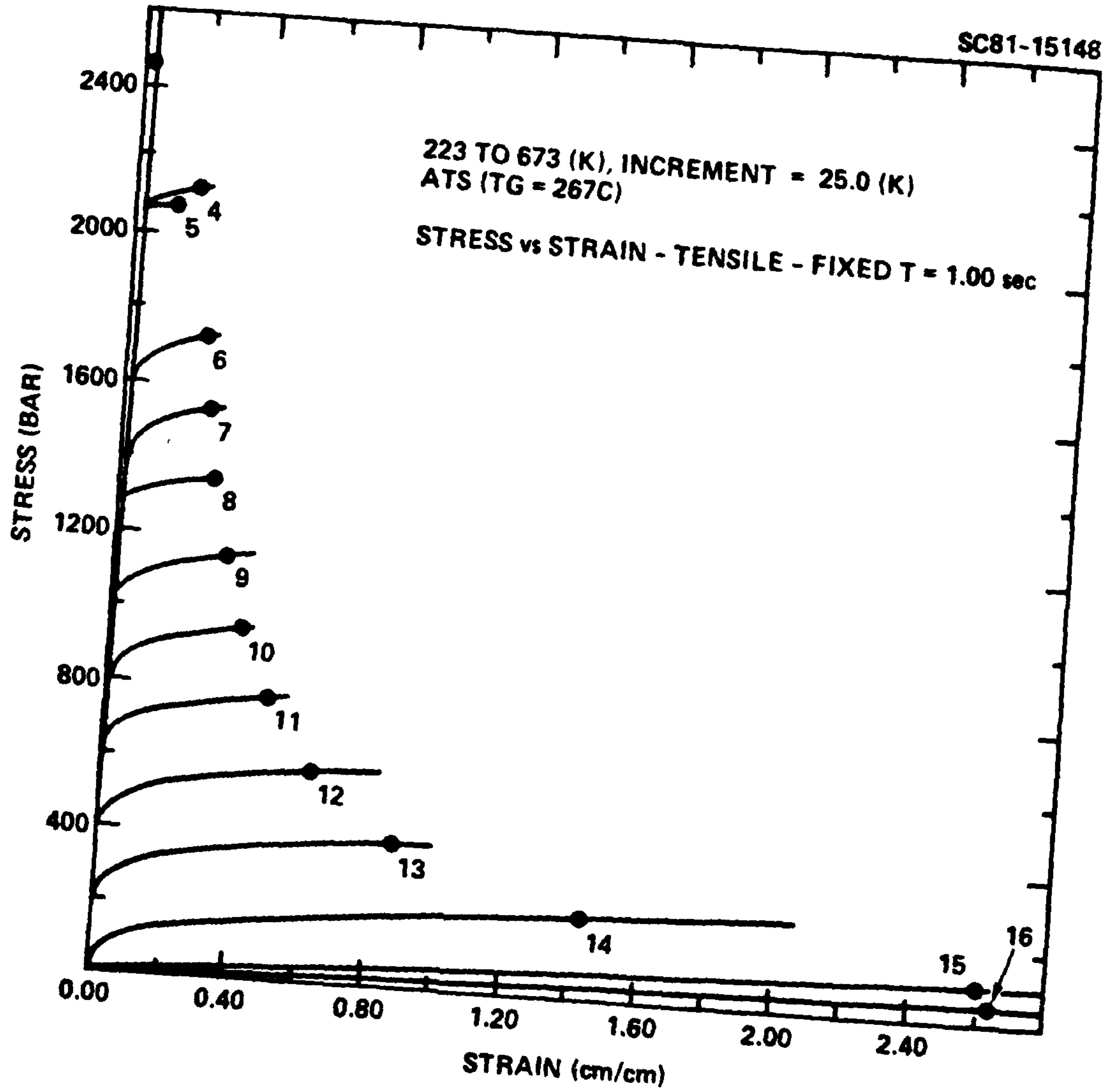


Fig. 4-10 Calculated curves of nominal tensile stress vs strain for linear ATS polymer with T_g = 267°C and M_p = 2.26E5 gm/mole (see Table 4-8 for temperatures).

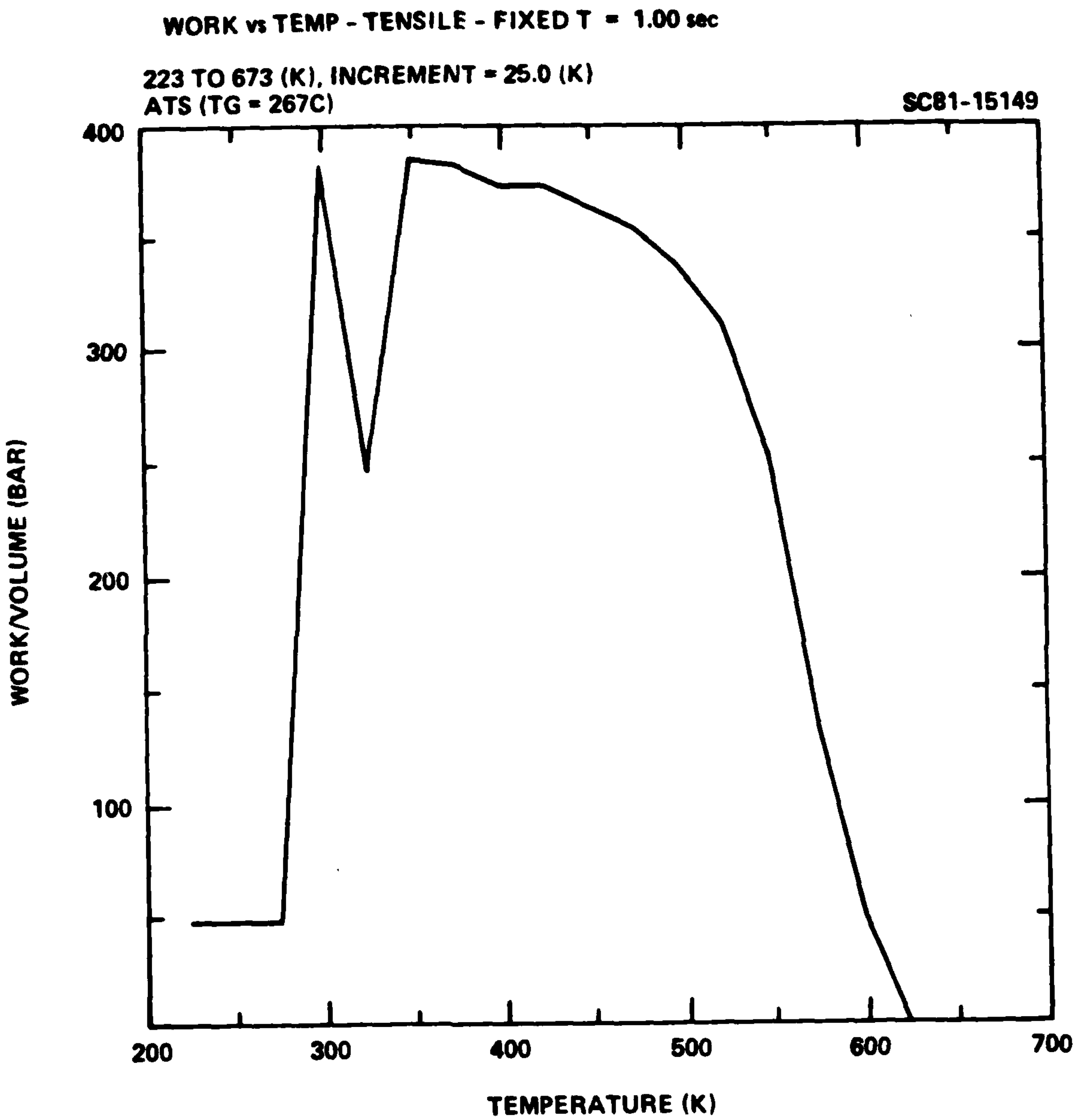


Fig. 4-11 Calculated temperature dependence of tensile fracture energy W_T per unit volume of unnotched linear ATS polymer.

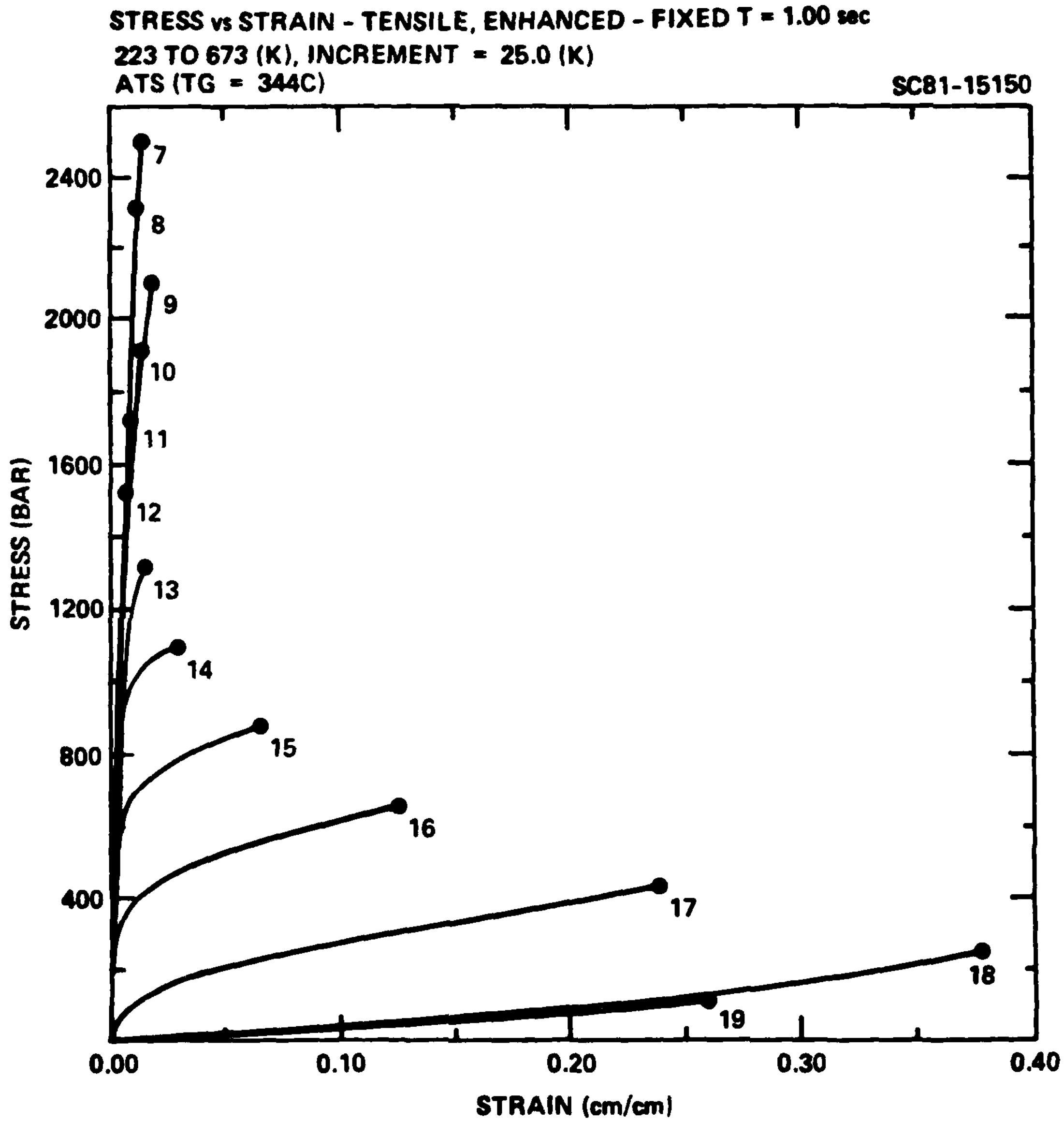


Fig. 4-12 Calculated curves of nominal tensile stress vs strain for crosslinked ATS with T_g = 344°C and M_p = 2.26E5 and M_c = 1817 gm/mole (see Table 4-8 for temperatures).

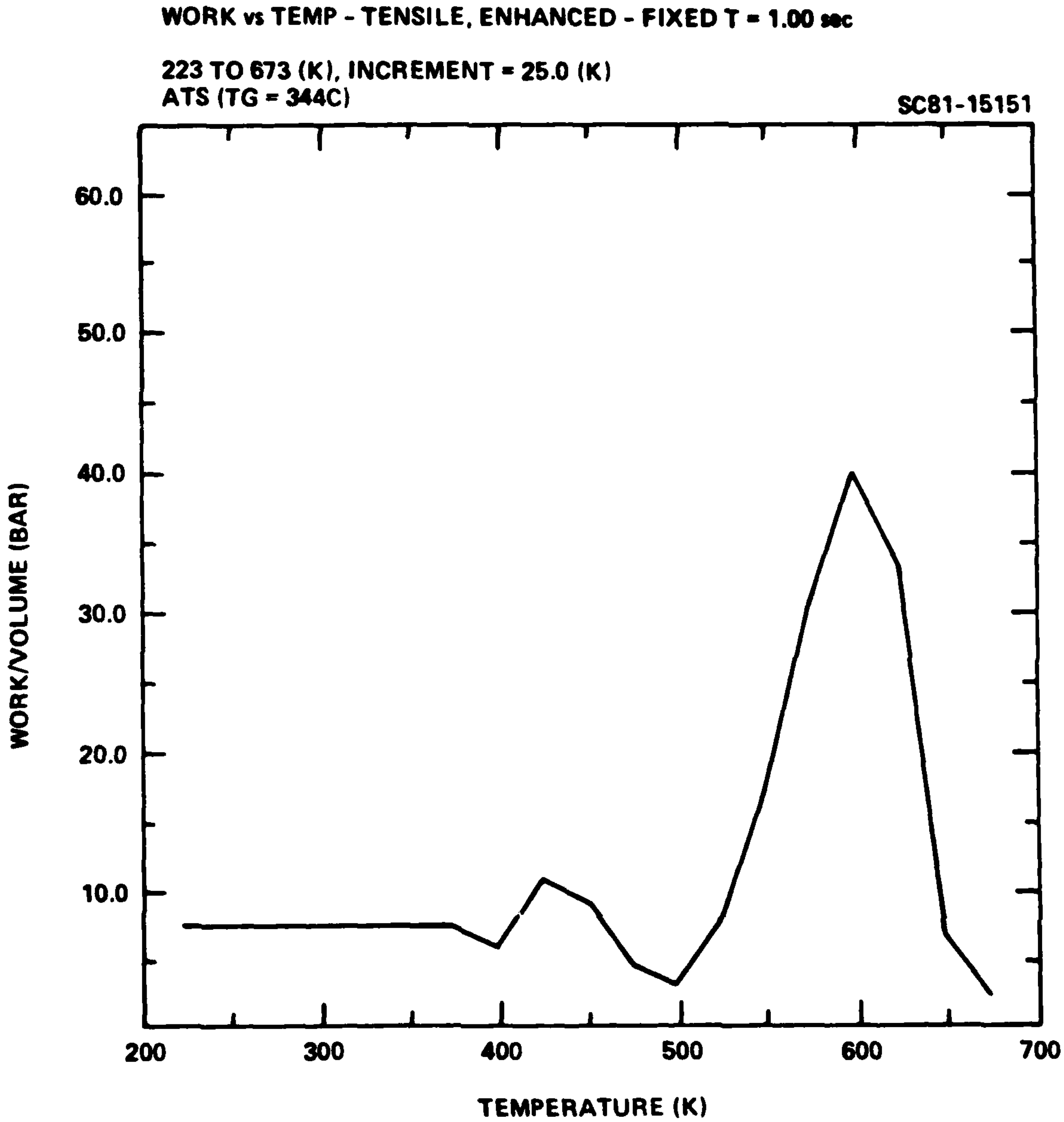


Fig. 4-13 Calculated temperature dependence of tensile fracture energy W_T per unit volume of unnotched crosslinked ATS polymer.

SC81-15152

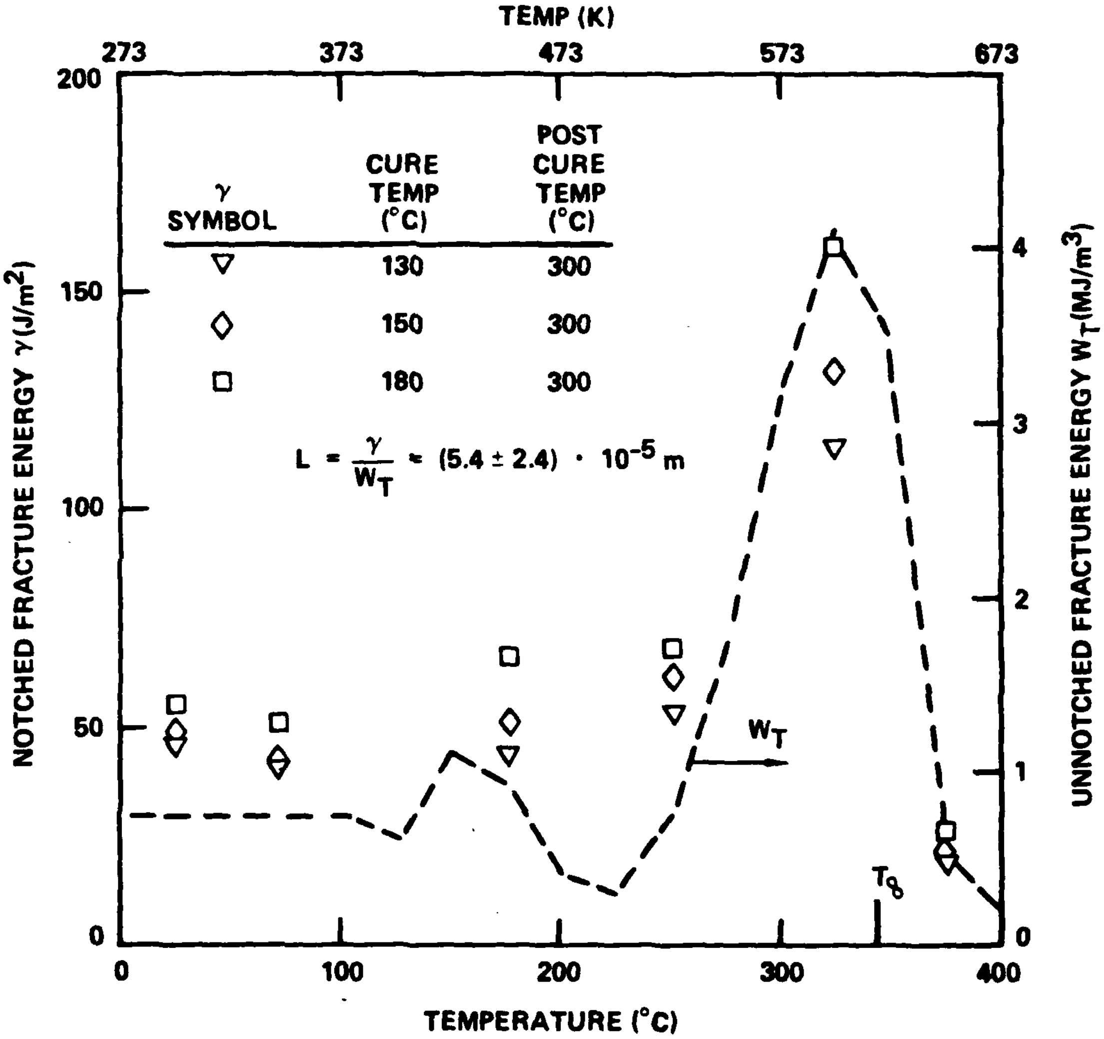


Fig. 4-14 Comparison of experimental notched fracture energy (γ) with unnotched fracture energy W_T from 25°C to 375°C.

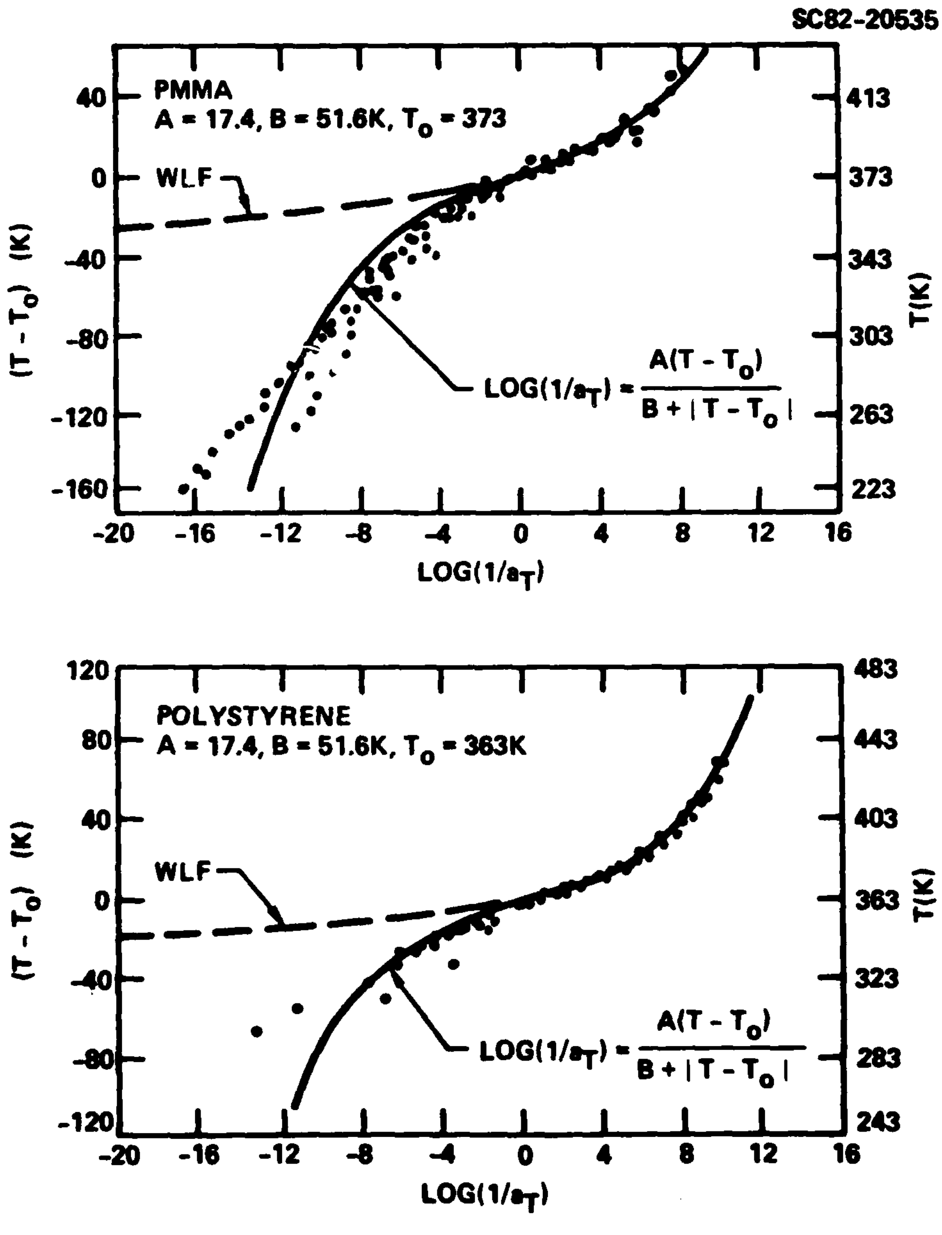
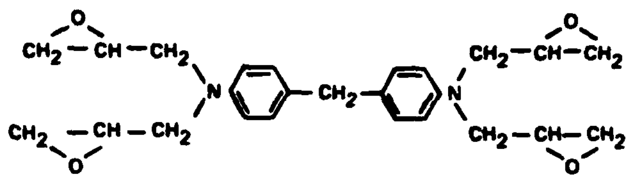
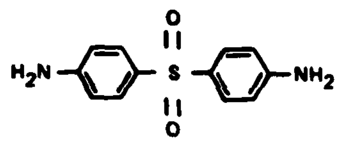


Fig. 4-15 Comparison of standard (dashed) and revised (solid curve) forms of WLF equations. (For summary of experimental time-temperature shift factors a_T, see Ref. 31, 32).

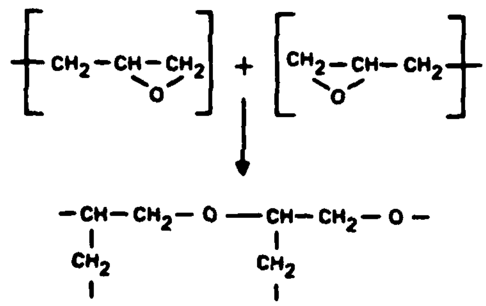
EPOXY (E): TETRAGLYCIDYL METHYLENE DIANILINE (TGMDA); M. W. ≅ 422 gm/MOLE   SC82-20340



CURATIVE (C): DIAMINODIPHENYLSULFONE (DDS); M. W. ≅ 248 GM/MOLE



CROSSLINK REACTION 1: (100% BY WEIGHT E)



CROSSLINK REACTION 2: (63% BY WEIGHT E + 37% BY WEIGHT C)

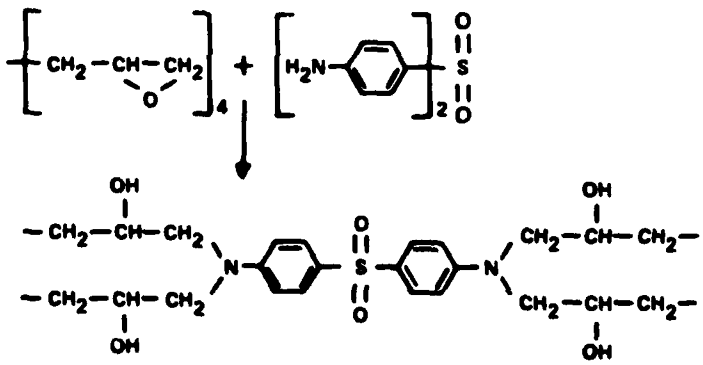


Fig. 5-1   Composition and suggested curing mechanisms for 177°C (350°F) service temperature epoxy resins.

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SC82-20342

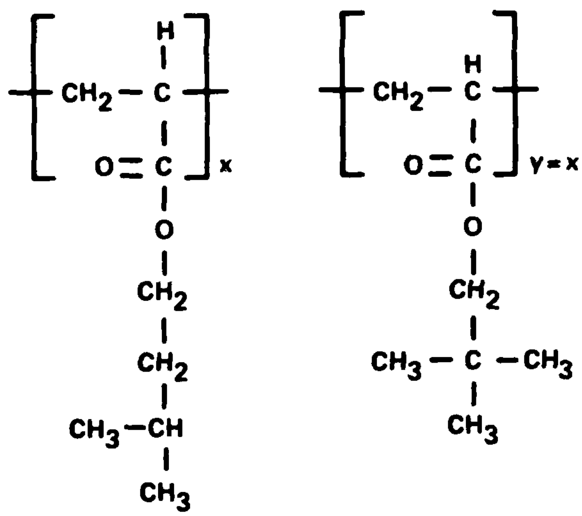


Fig. 5-2 Repeat structure for 50:50 mole % isoamyl acrylate = Neopentyl acrylate of number average molecular weight M_n = 1.03E6 g/mol, V_p (230K) = 1.01 cc/gm, T_g = 230K, and M_e = 21,000 gm/mole.

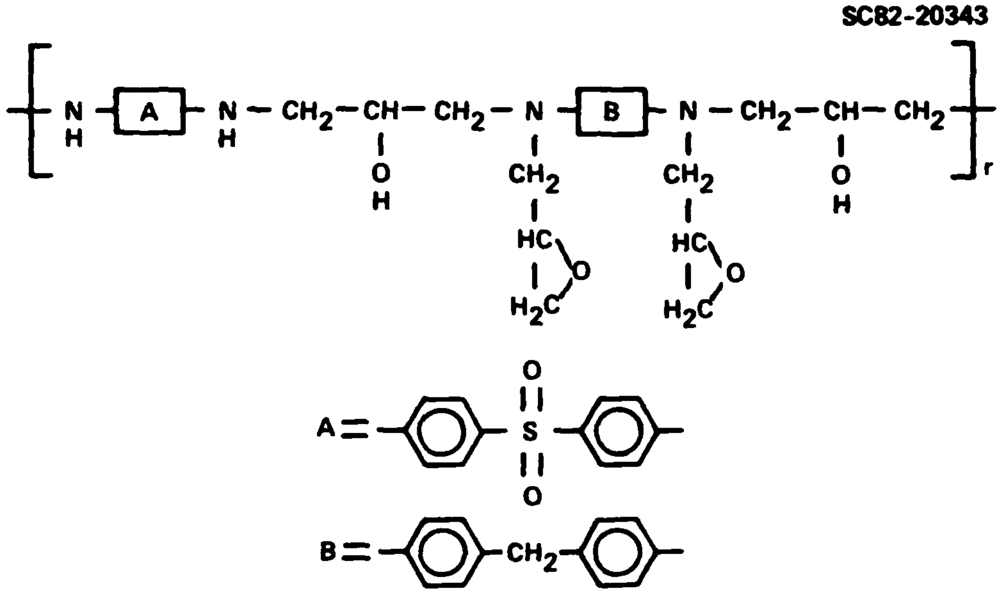


Fig. 5-3 Molecular structure of equimolar amounts of TGMDA and (37 wt%) DDS polymerized by chain extension.

SC82-20344

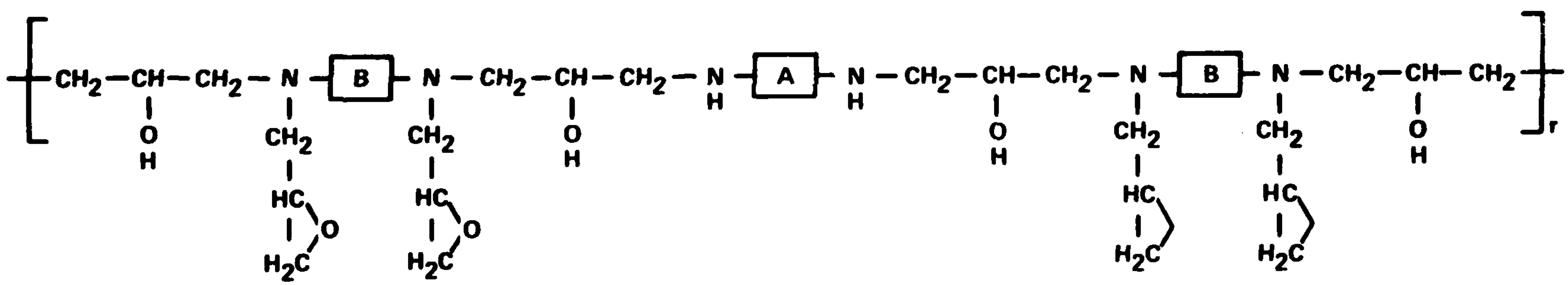


Fig. 5-4 Molecular structure of 2 moles TGMDA and 1 mole (22.7 wt%) DDS polymerized by chain extension.

SC82-20341

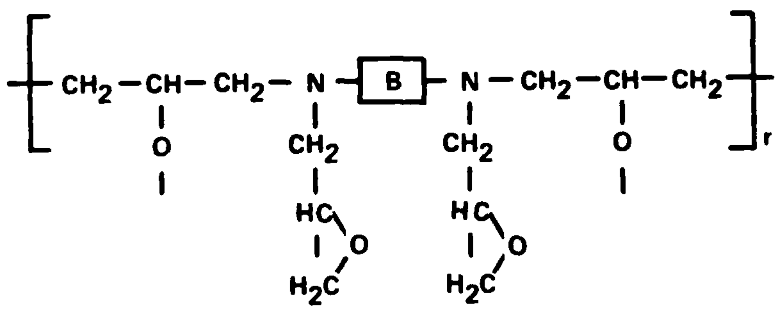


Fig. 5-5 Molecular structure of chain extended TGMDA homopolymer.

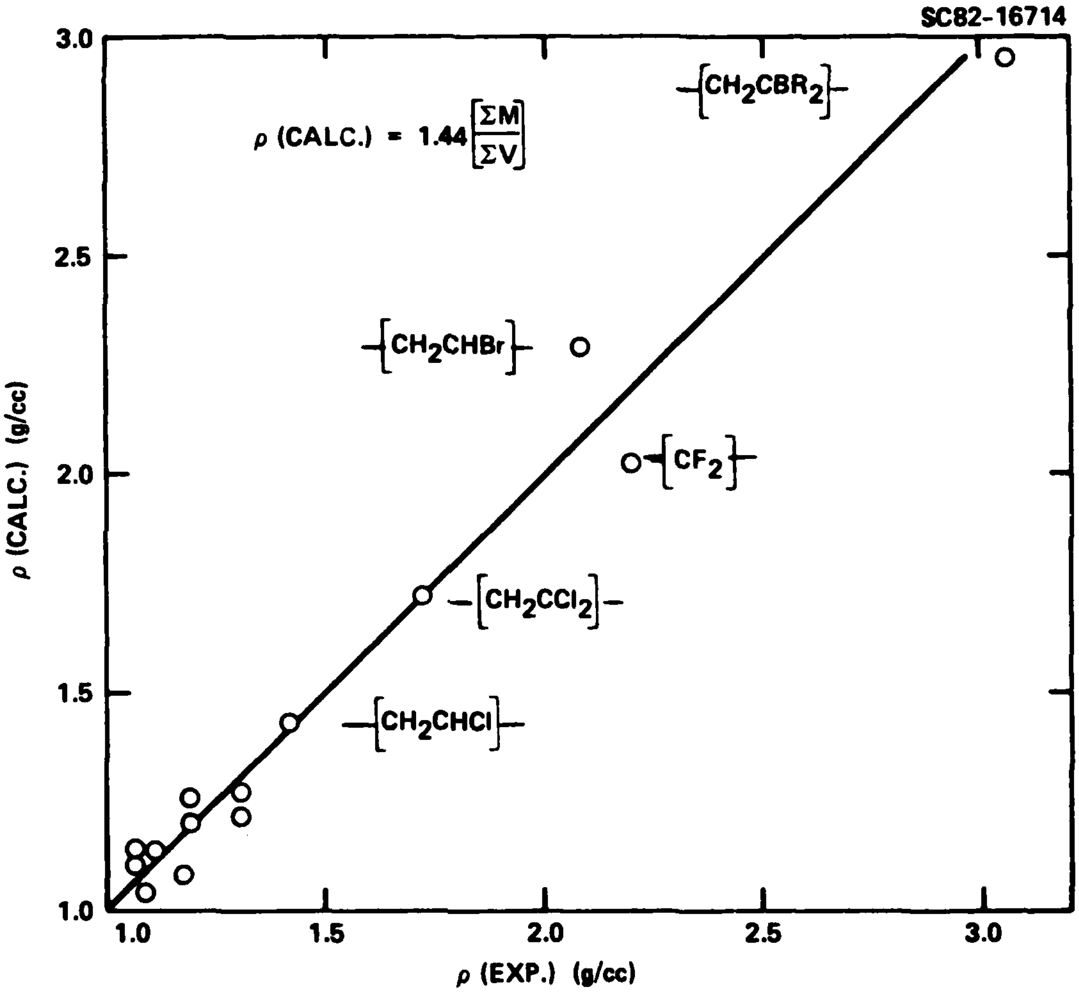


Fig. 5-6 Comparison of calculated and experimental density of solid polymers at 298K (data from Ref. 5).

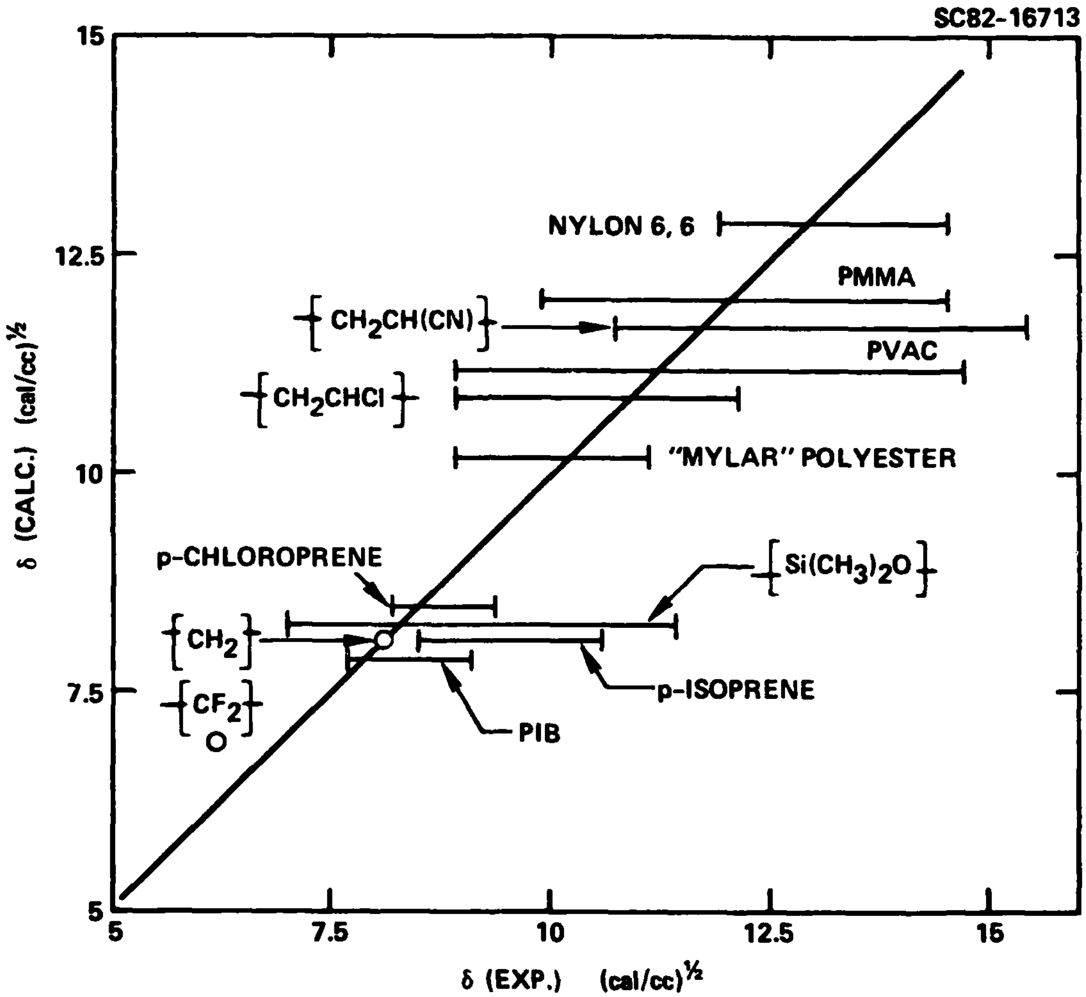


Fig. 5-7 Comparison of calculated and experimental solubility parameter (data from Refs. 9, 10).

SC82-16708

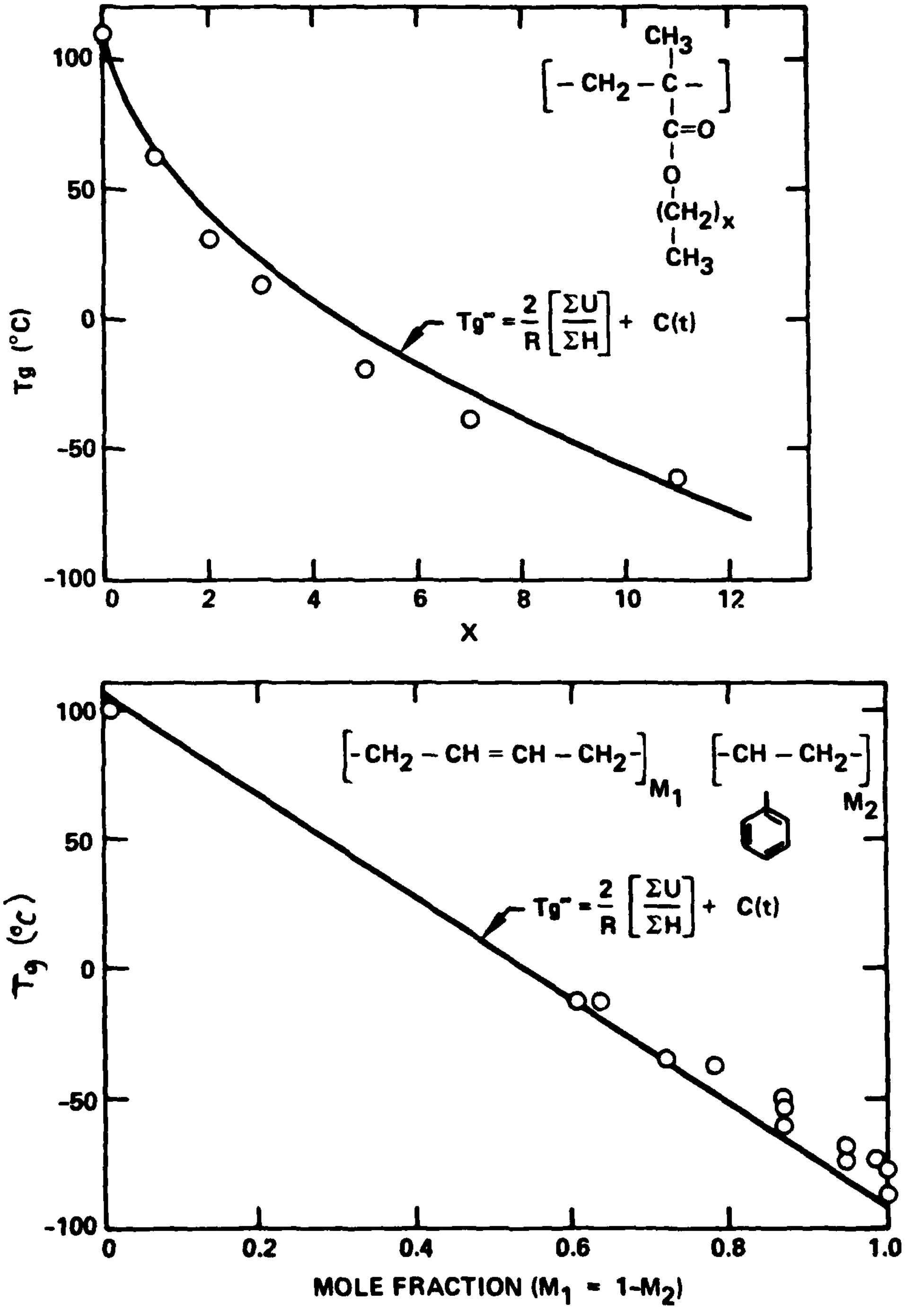


Fig. 5-8 Comparison of calculated and experimental glass temperatures for polyacrylates (upper curve) and butadiene-styrene copolymers (Refs. 11, 12).

SC82-16712

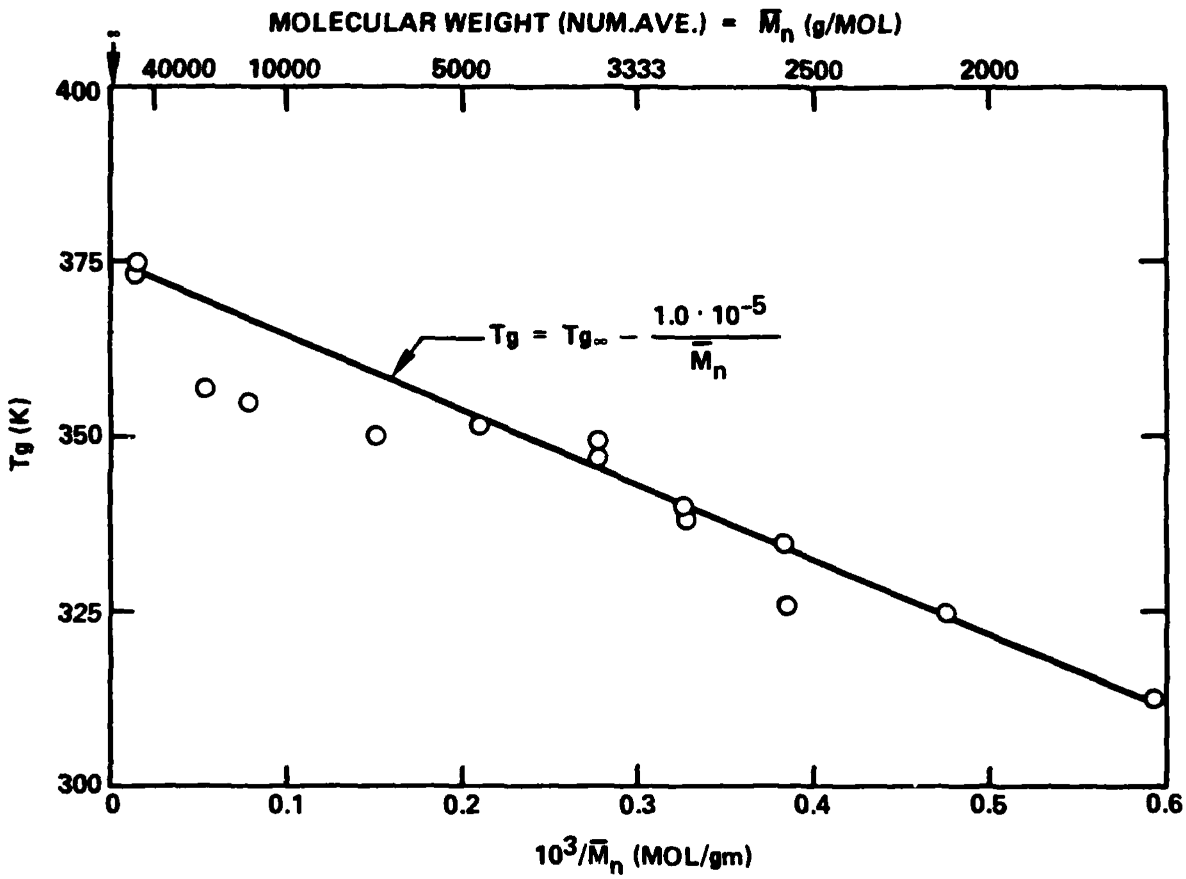


Fig. 5-9 M_n vs T_g for atactic polystyrene (data from Refs. 13, 14).

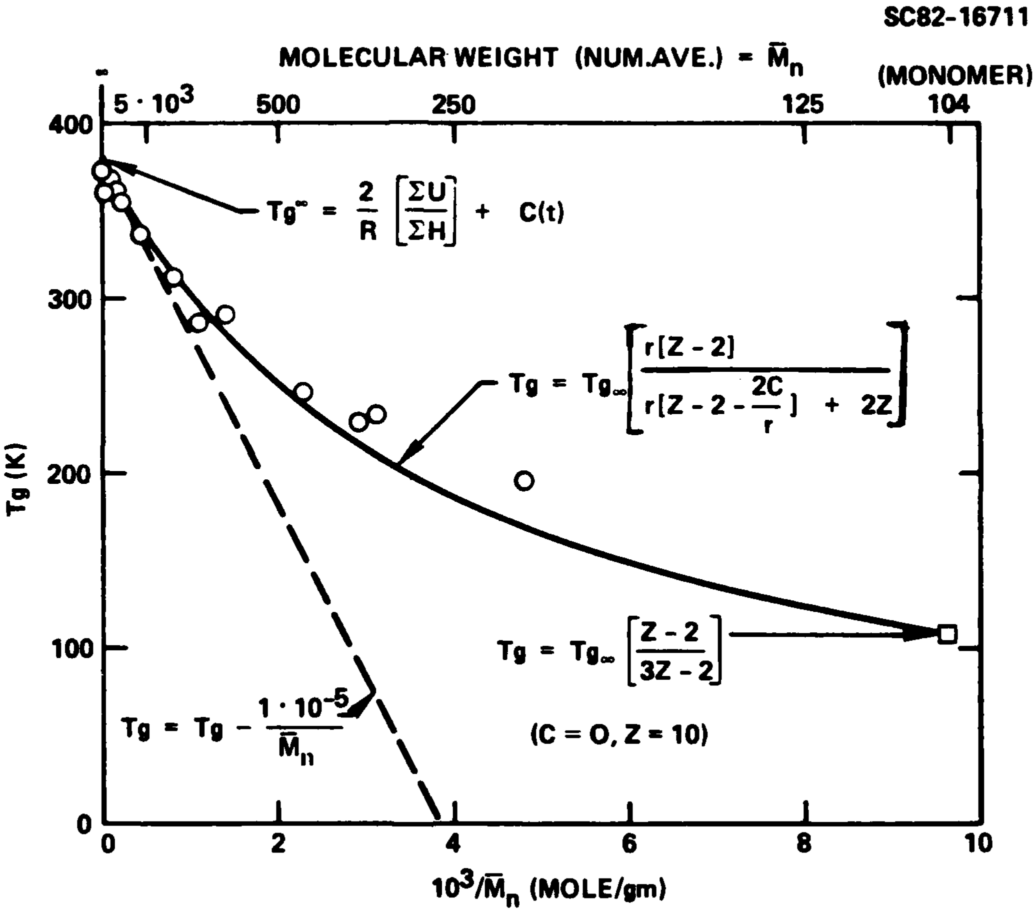


Fig. 5-10 M_n vs T_g for atactic polystyrene (data from Refs. 15, 16).

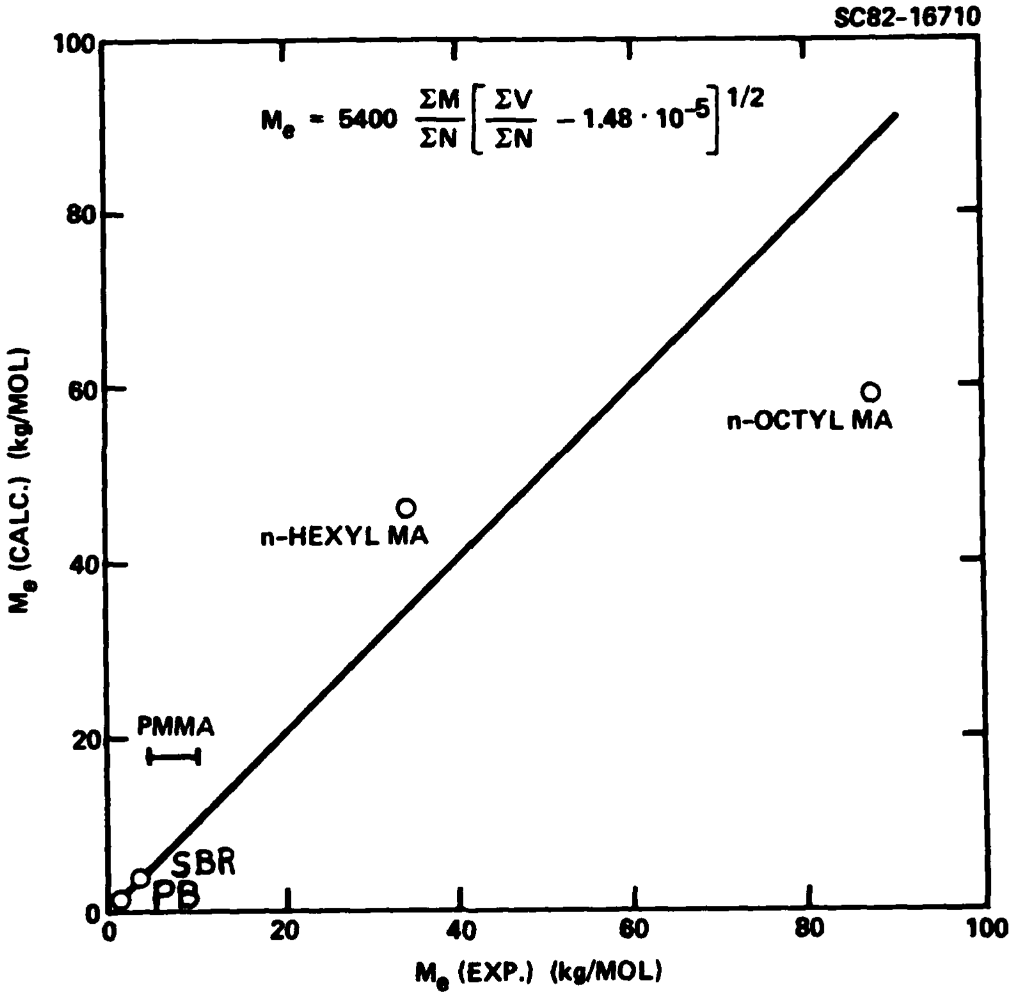


Fig. 5-11 Comparison of calculated and experimental entanglement molecular weight (data from Ref. 17).

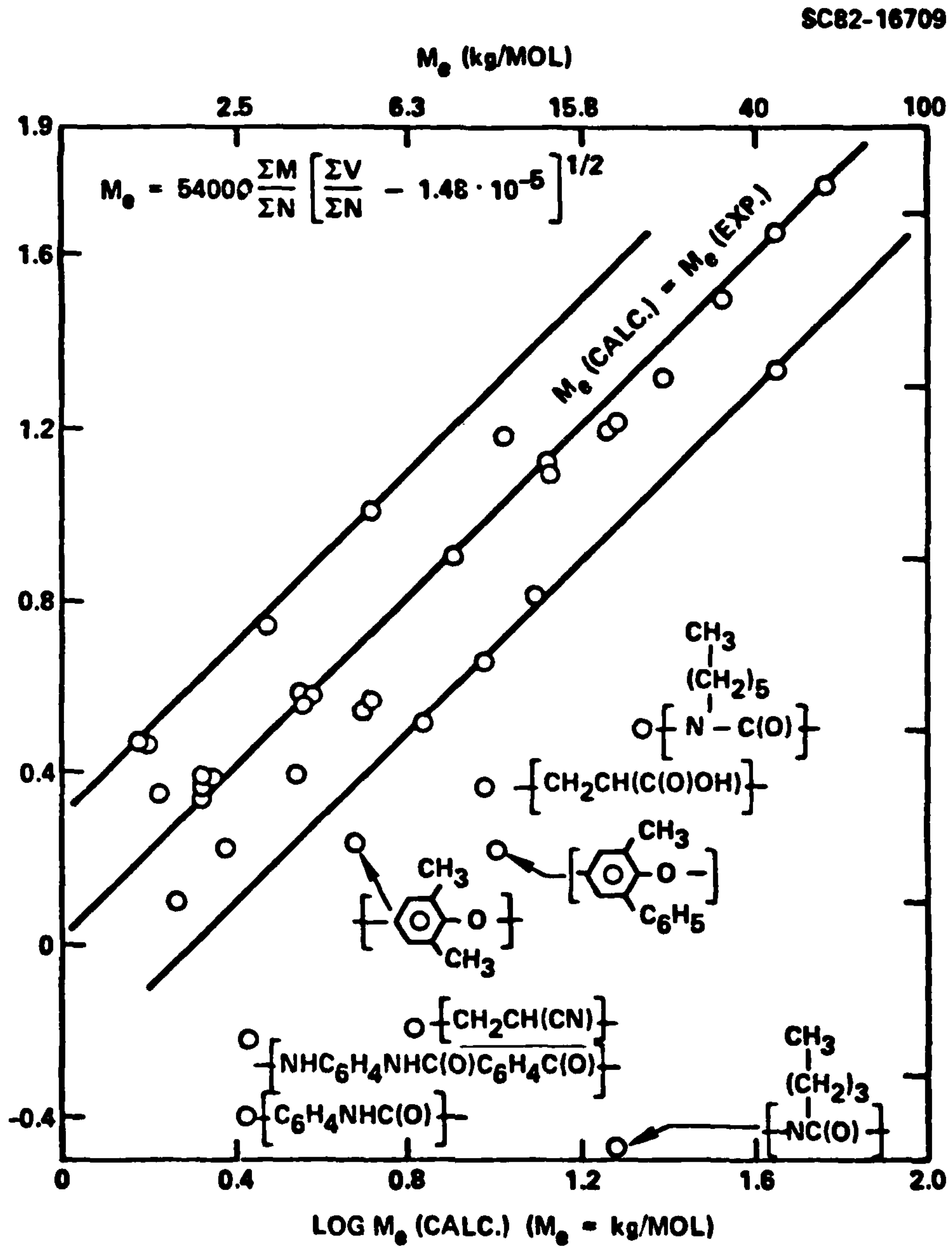


Fig. 5-12 Comparison of calculated and experimental entanglement molecular weight (data from Ref. 18).

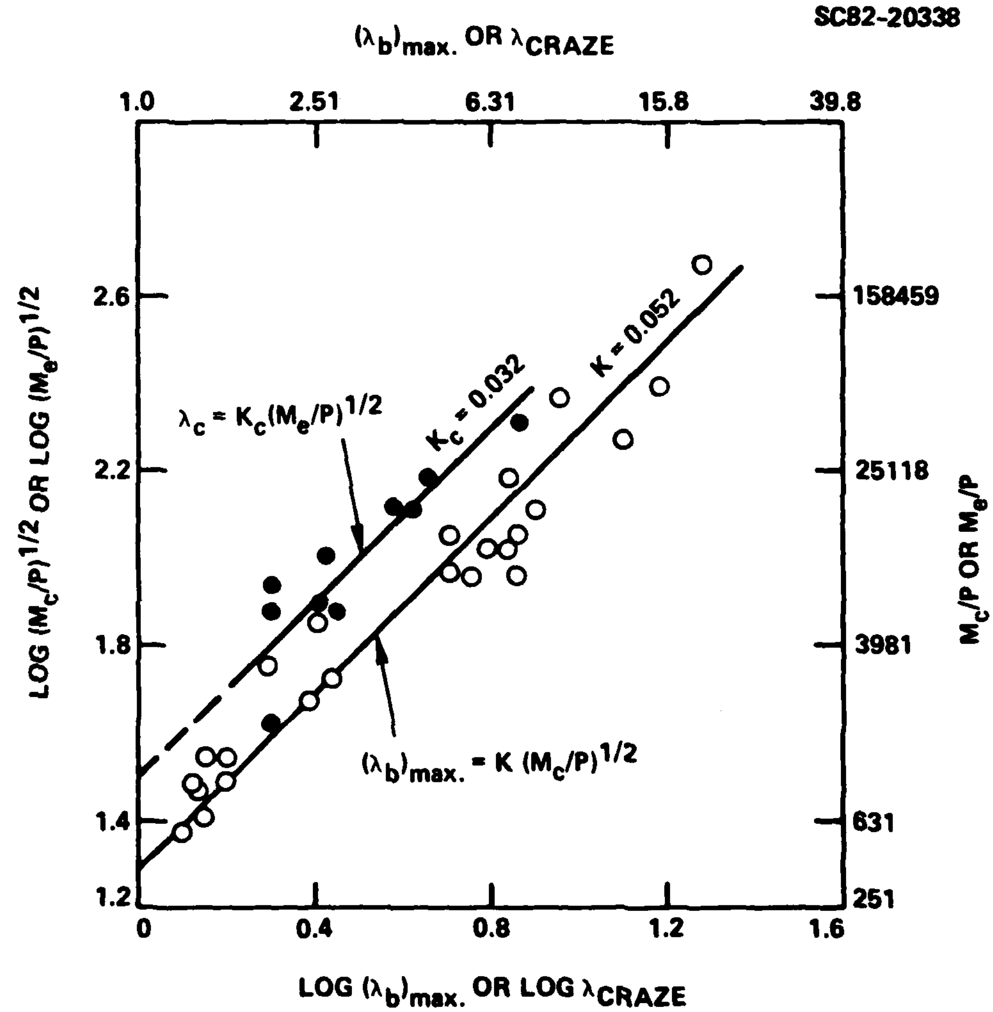


Fig. 5-13 Correlation between entanglement density (ρ/M_e) or chemical crosslink density (ρ/M_c) and maximum extension ratio λ_b or maximum craze extensibility λ_{craze}.

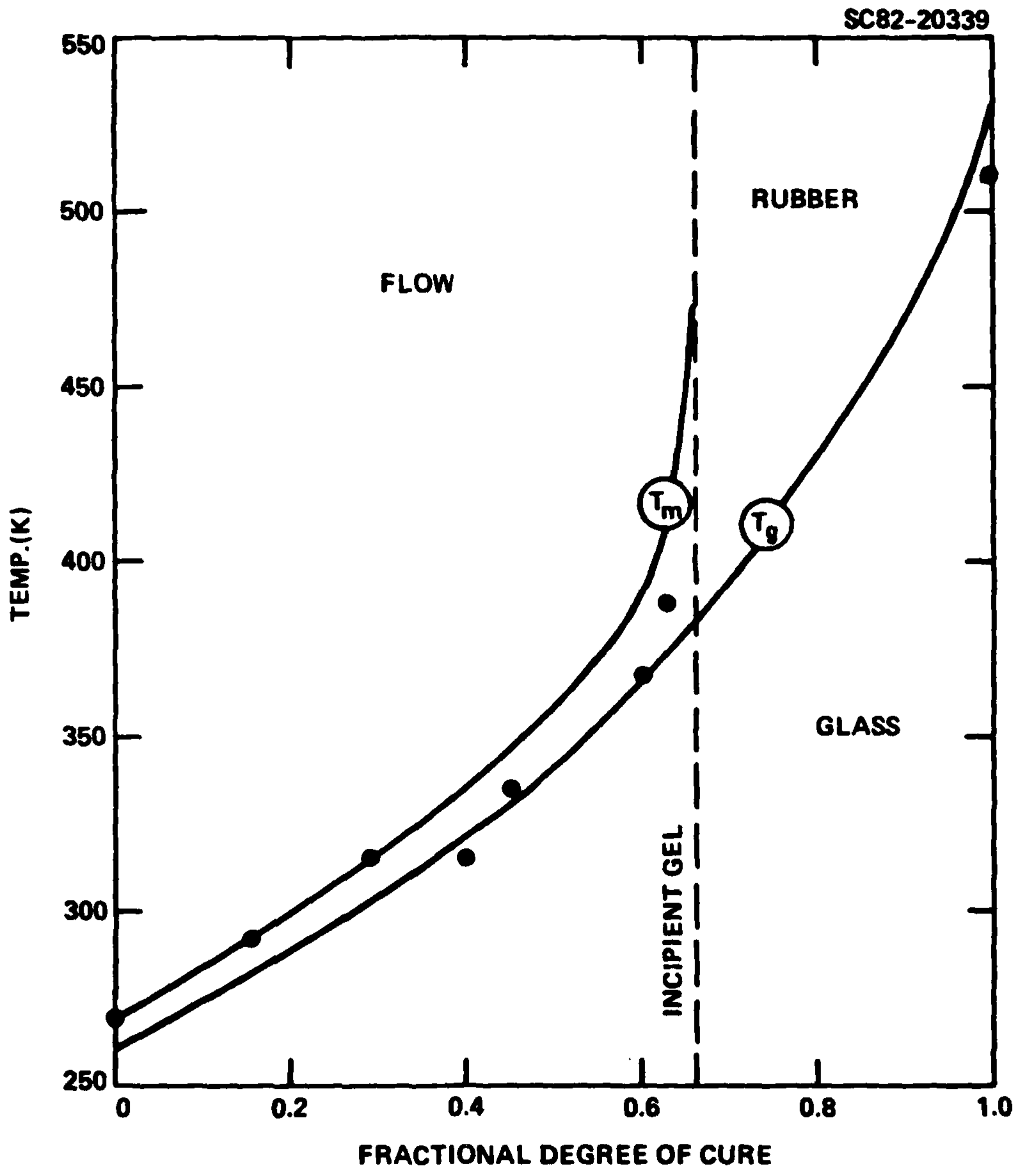


Fig. 5-14 Comparison of computed T_g and T_m curves for nonstoichiometric TGMDA/DDS (see Table 5-22) and measured T_g (X's) for Hercules 3501-5 epoxy resin (see Table 1-6 and Ref. 44).

SC82-20430

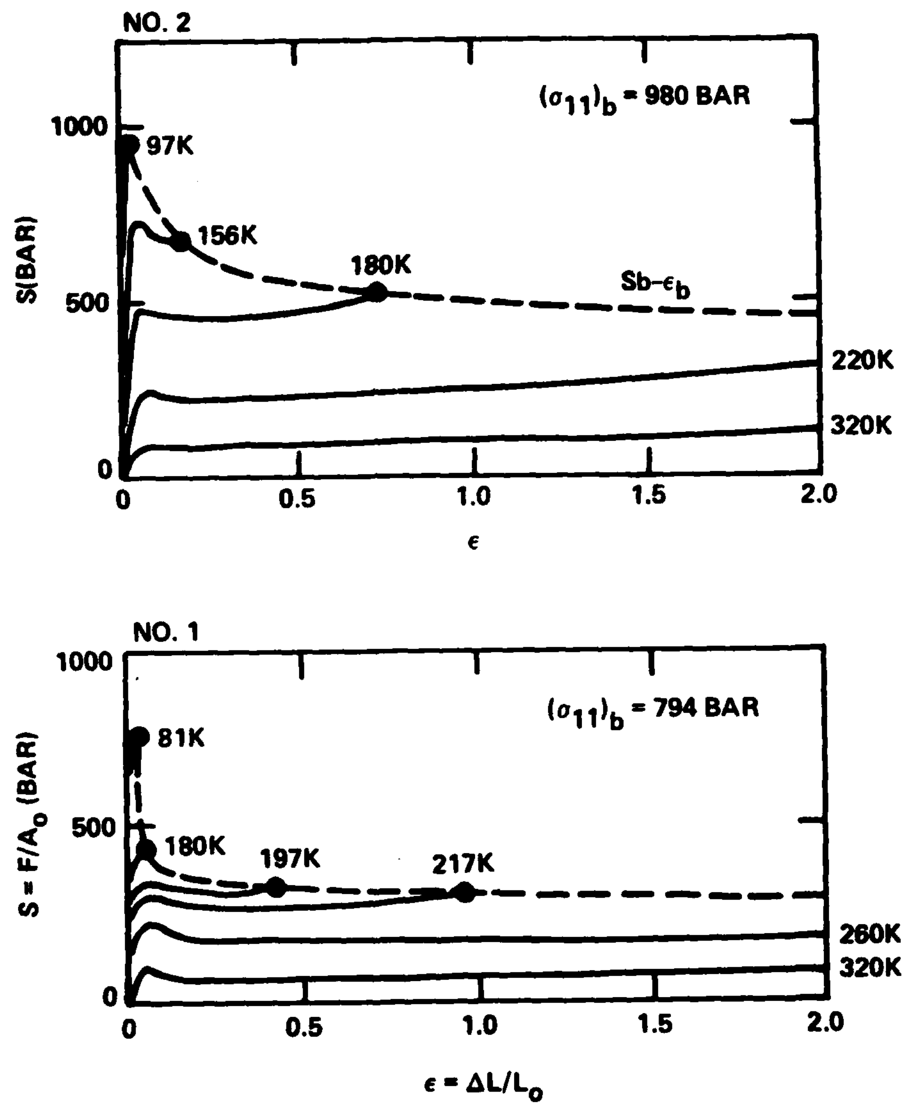


Fig. 6-1 Tensile response of C_2F_4 homopolymer (lower view) and $(C_2F_4)_{1.0}$ $(C_3F_6)_{0.14}$ copolymer (upper view) films.

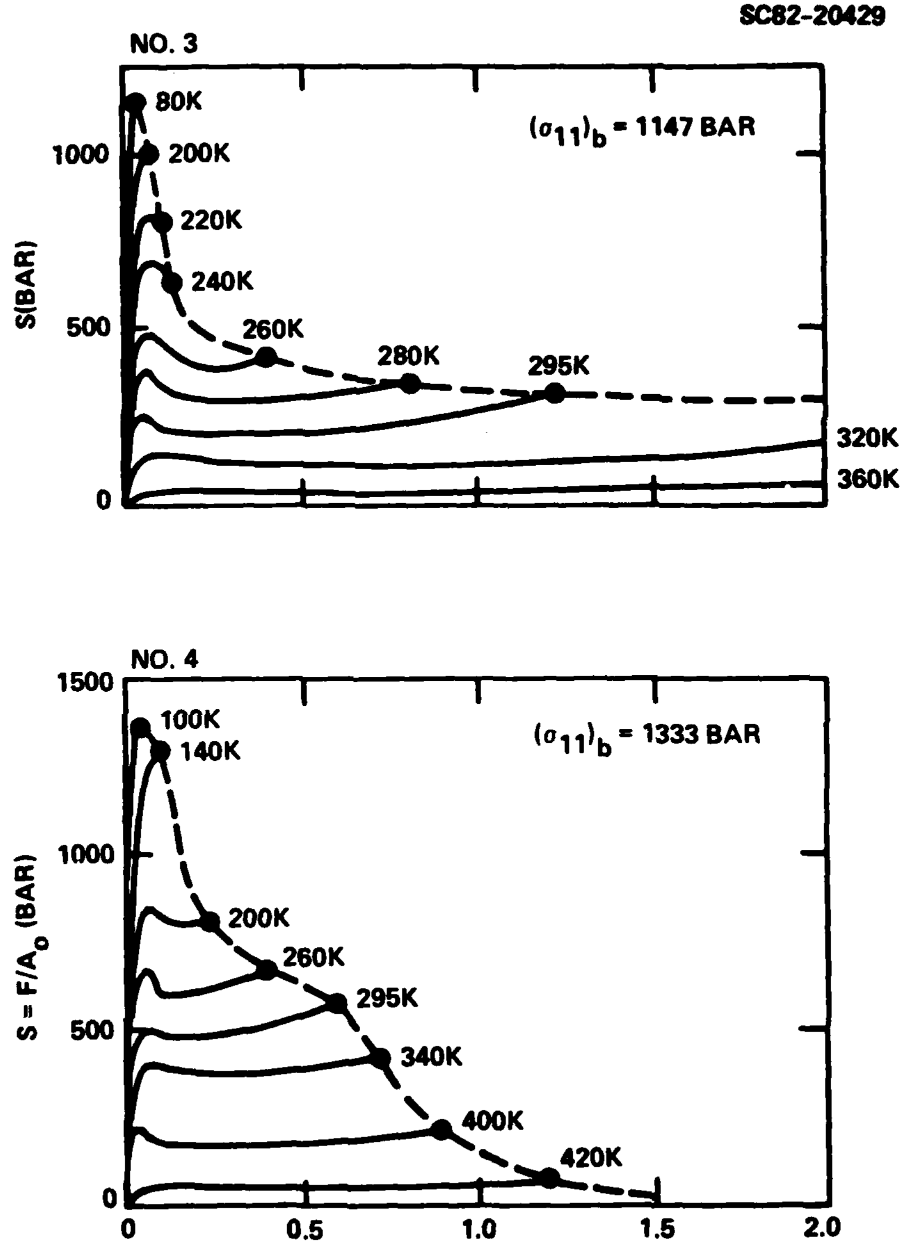


Fig. 6-2 Tensile response of $(CF_2CFCL)_{1.0}$ $(CF_2CH_2)_{0.03}$ copolymer (upper view) and polybisphenol-A carbonate (lower view) films.

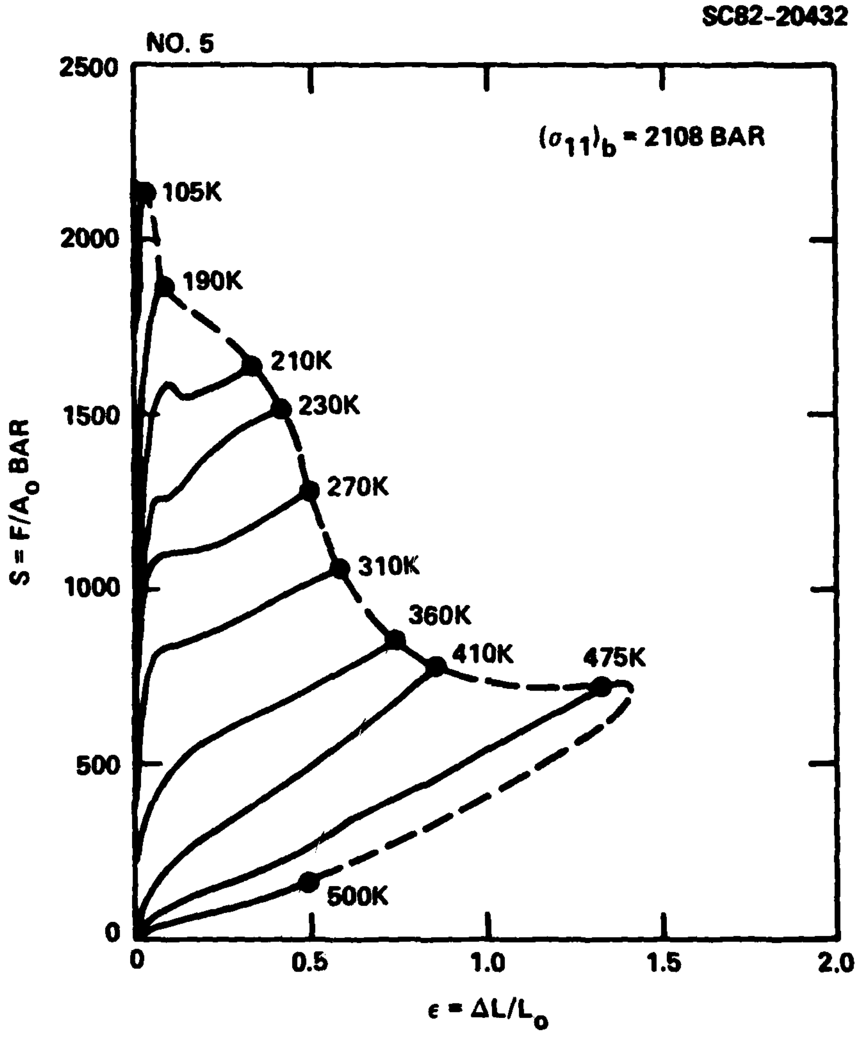


Fig. 6-3 Tensile response of polyethyleneterephthalate film.

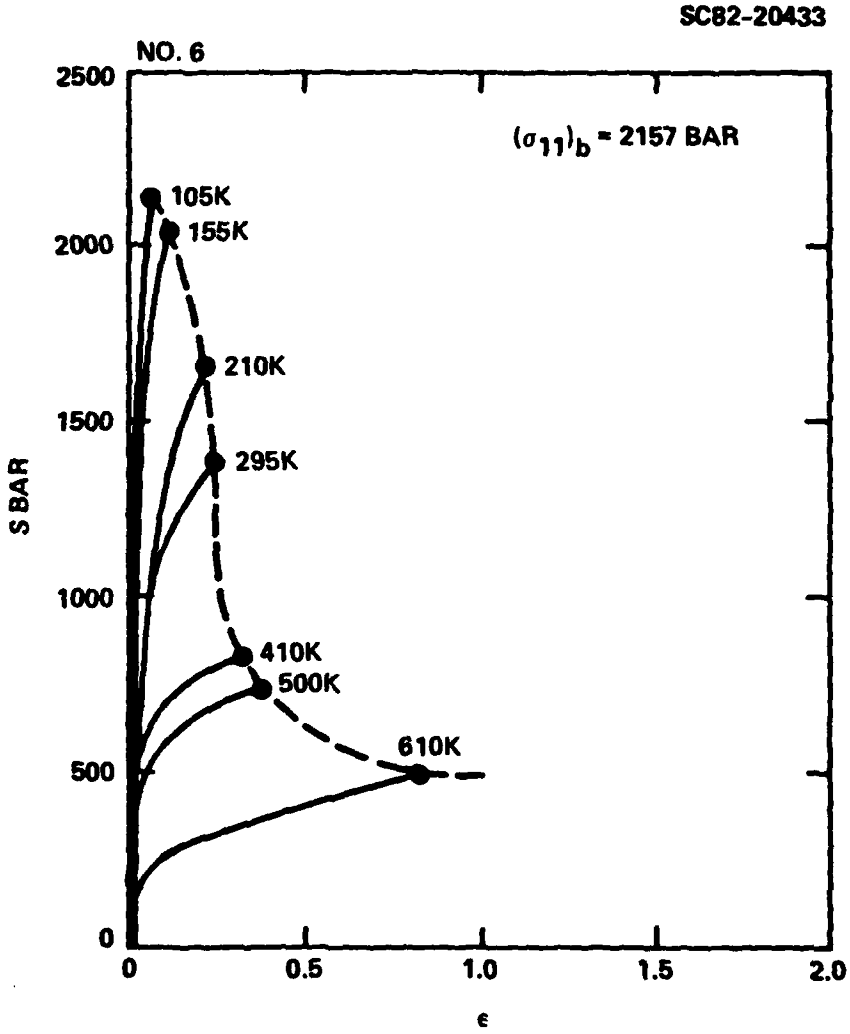


Fig. 6-4 Tensile response of $(N(CO)_2\ C_6H_2(CO)_2NC_6H_4OC_6H_4)$ polyimide film.

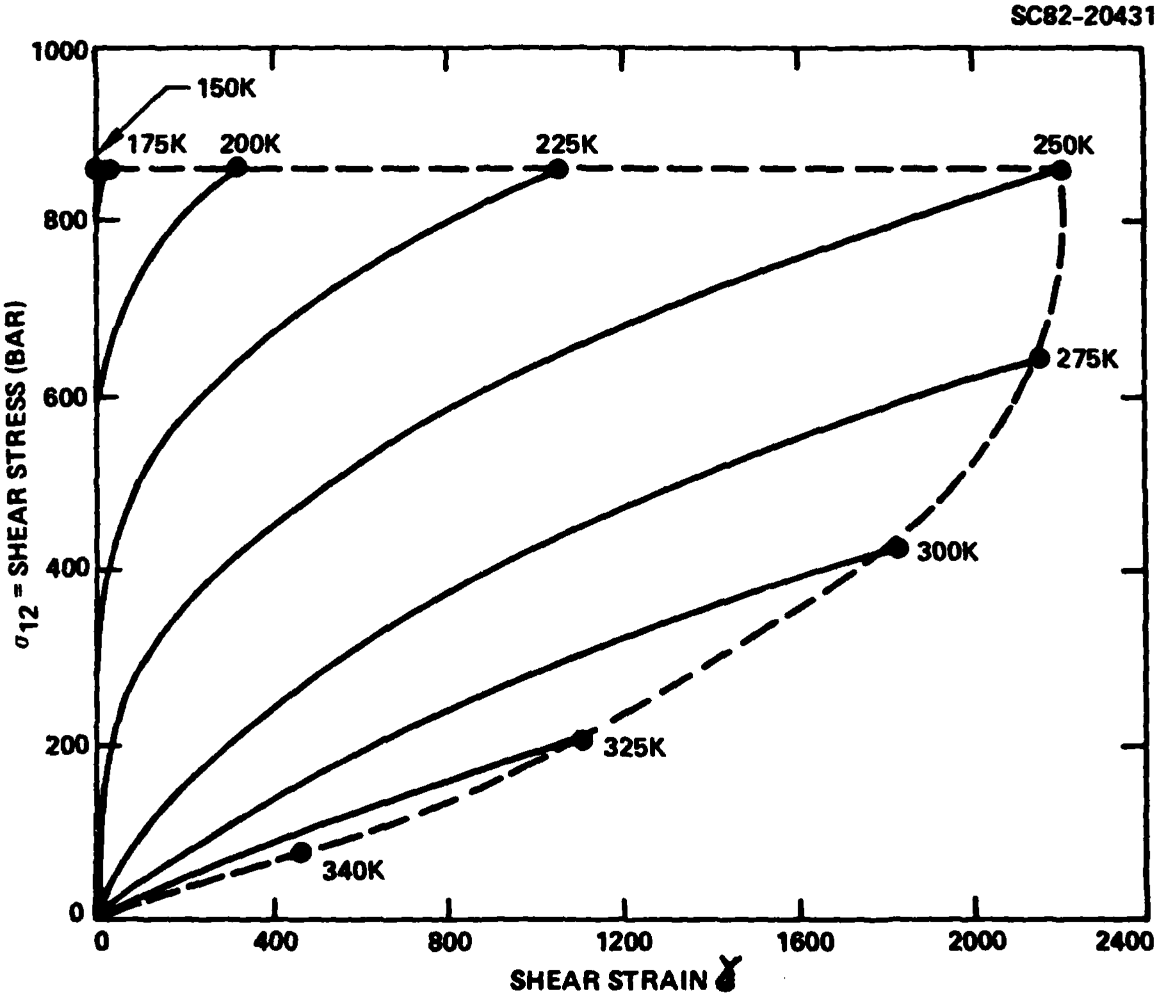


Fig. 6-5 Calculated shear stress vs strain response for equimolar isoamyl-neopentyl acrylate copolymer (M_n = 1.03E6 g/mol, T_g = 230K).

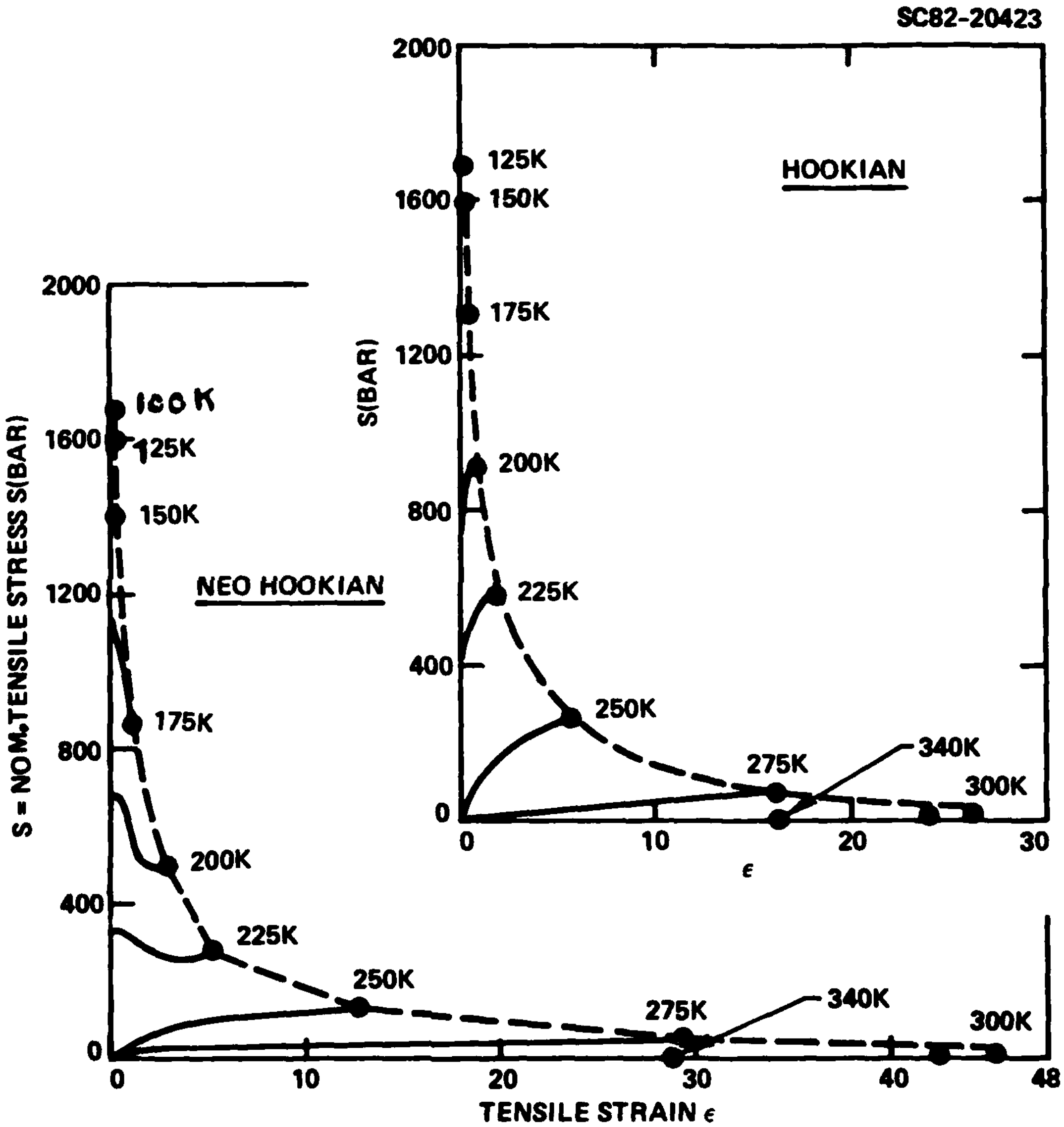


Fig. 6-6 Calculated tensile stress vs strain response for equimolar isoamyl-neopentyl acrylate copolymer (M_n = 1.03E6 g/mol, T_g = 230K).

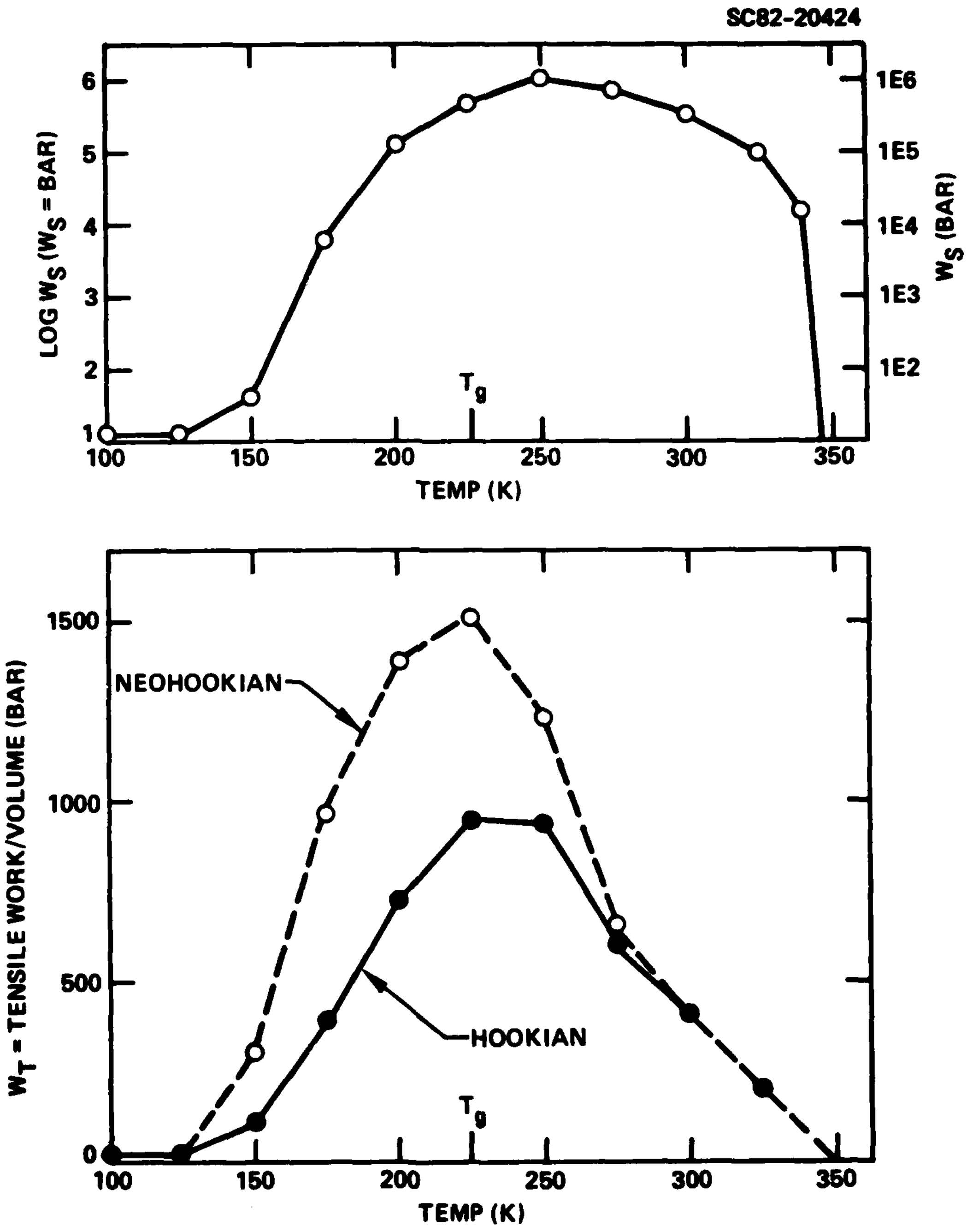


Fig. 6-7 Calculated shear (upper view) and tensile (lower view) works of deformation per unit volume.

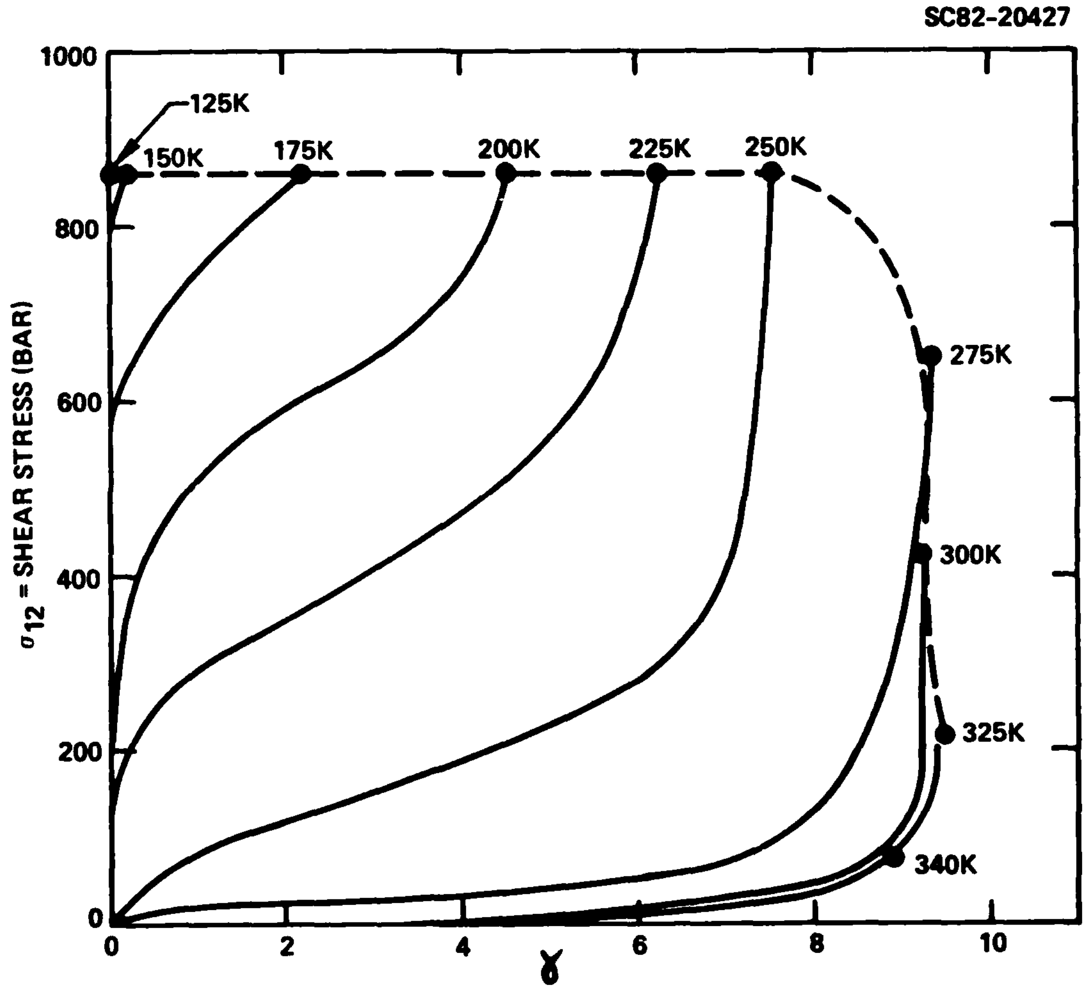


Fig. 6-8 Calculated shear stress vs strain response for equimolar isoamyl-neopentyl acrylate copolymer (M_n = 1.03E6 g/mol, T_g = 230K) with light crosslinking (M_c = 3.42E4 g/mol).

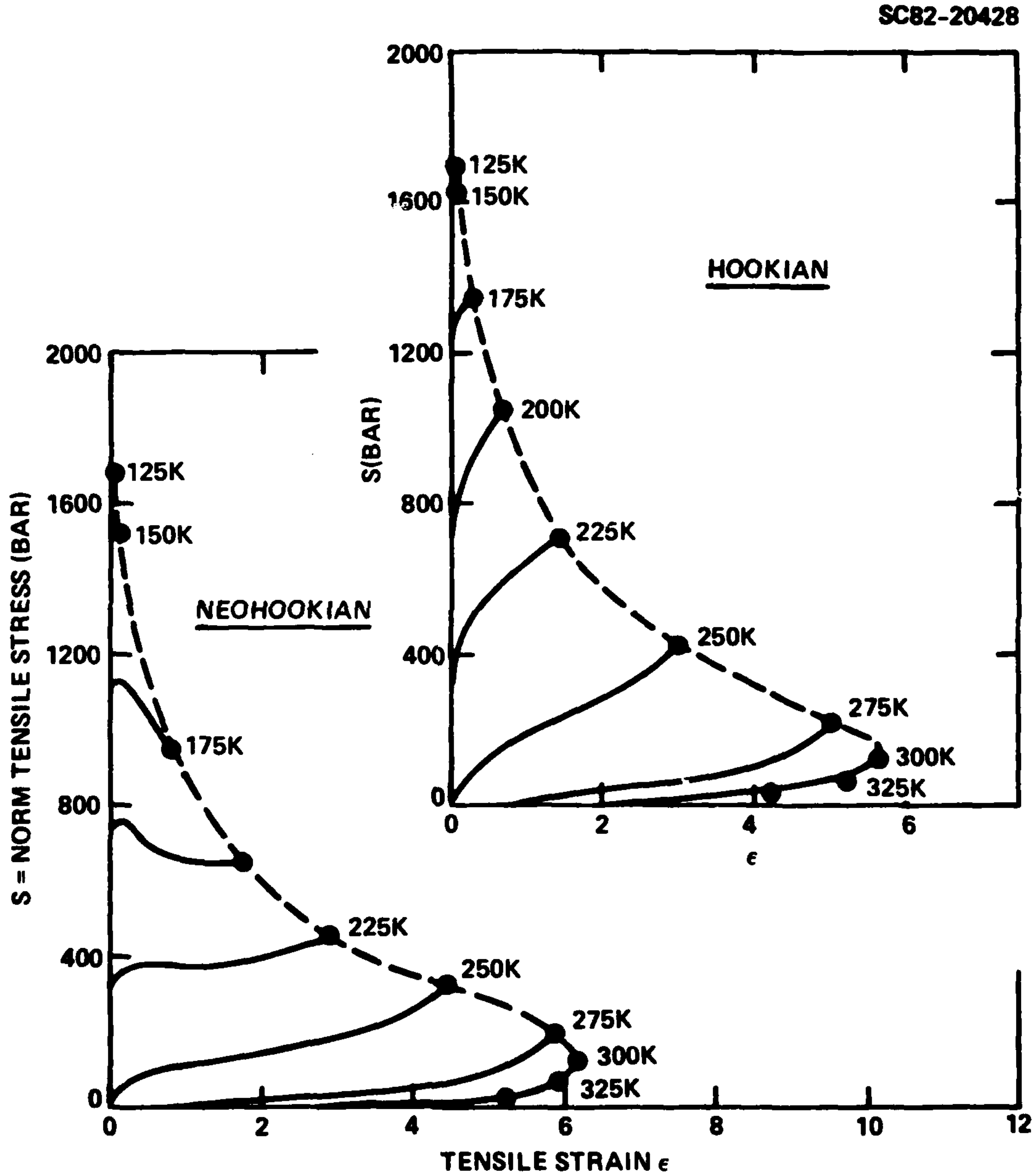


Fig. 6-9 Calculated tensile stress vs strain response for equimolar isoamyl-neopentyl copolymer (M_n = 1.06E6 g/mol, T_g = 230K) and light crosslinking (M_c = 3.42E4 g/mol).

SC82-20426

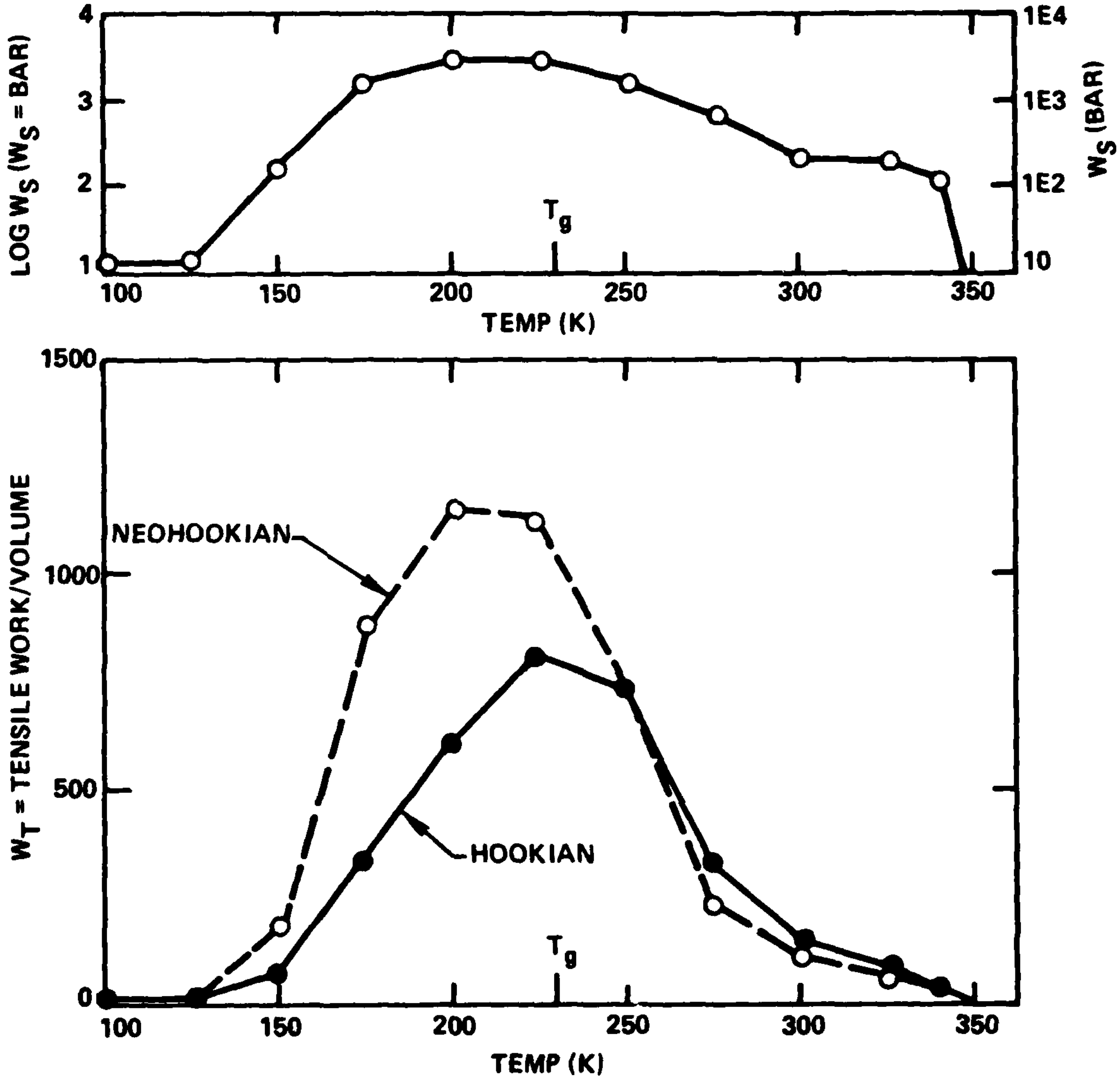


Fig. 6-10 Calculated shear (upper view) and tensile (lower view) works of deformation per unit volume.

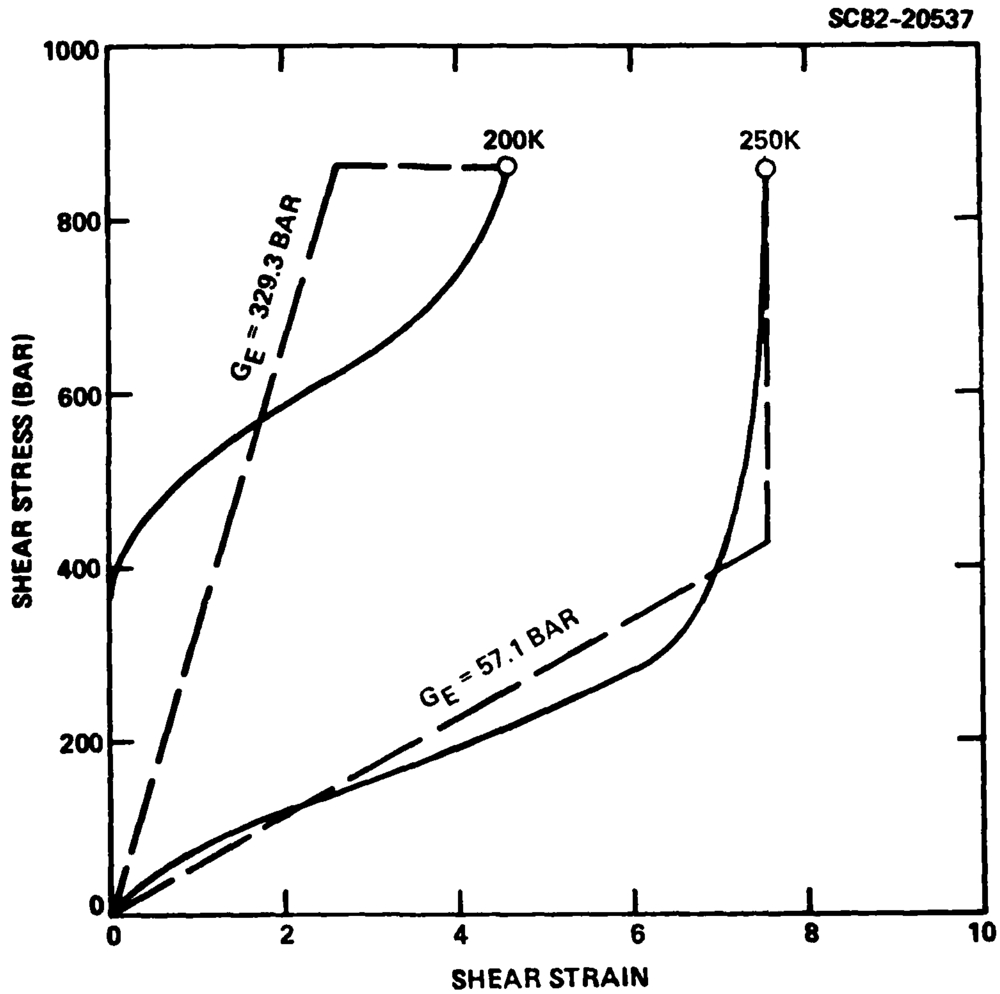


Fig. 6-11 Calculated shear stress vs strain (solid curves) response (see Fig. 6-8) and elastic-plastic analogs (dashed curves) for lightly crosslinked equimolar isoamyl-neopentyl acrylate copolymer.

SC82-24025

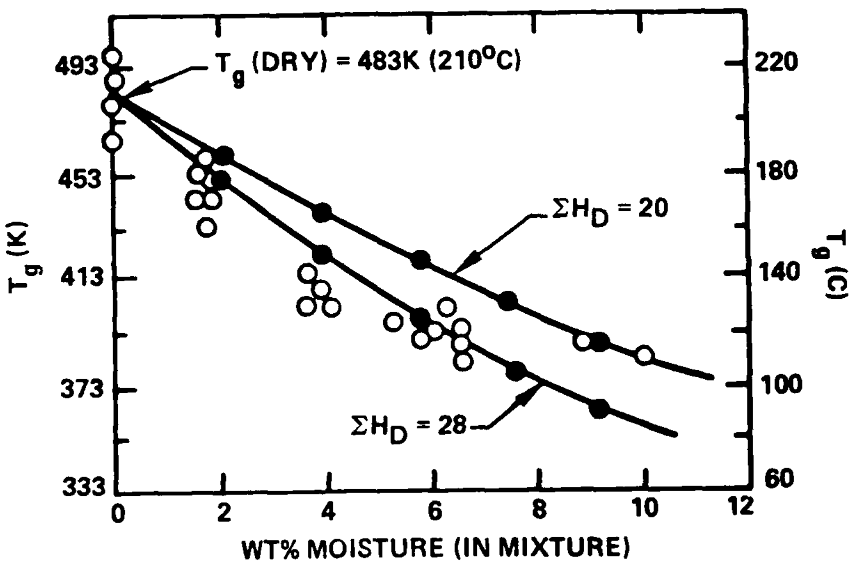


Fig. 6-12 Calculated (X) and experiment (•) effects of moisture on T_g of six cured epoxy resins (3501-5, 3501-6, 5208, 934, 3502, and NMD 2373); (for data see Ref. 6, 36).

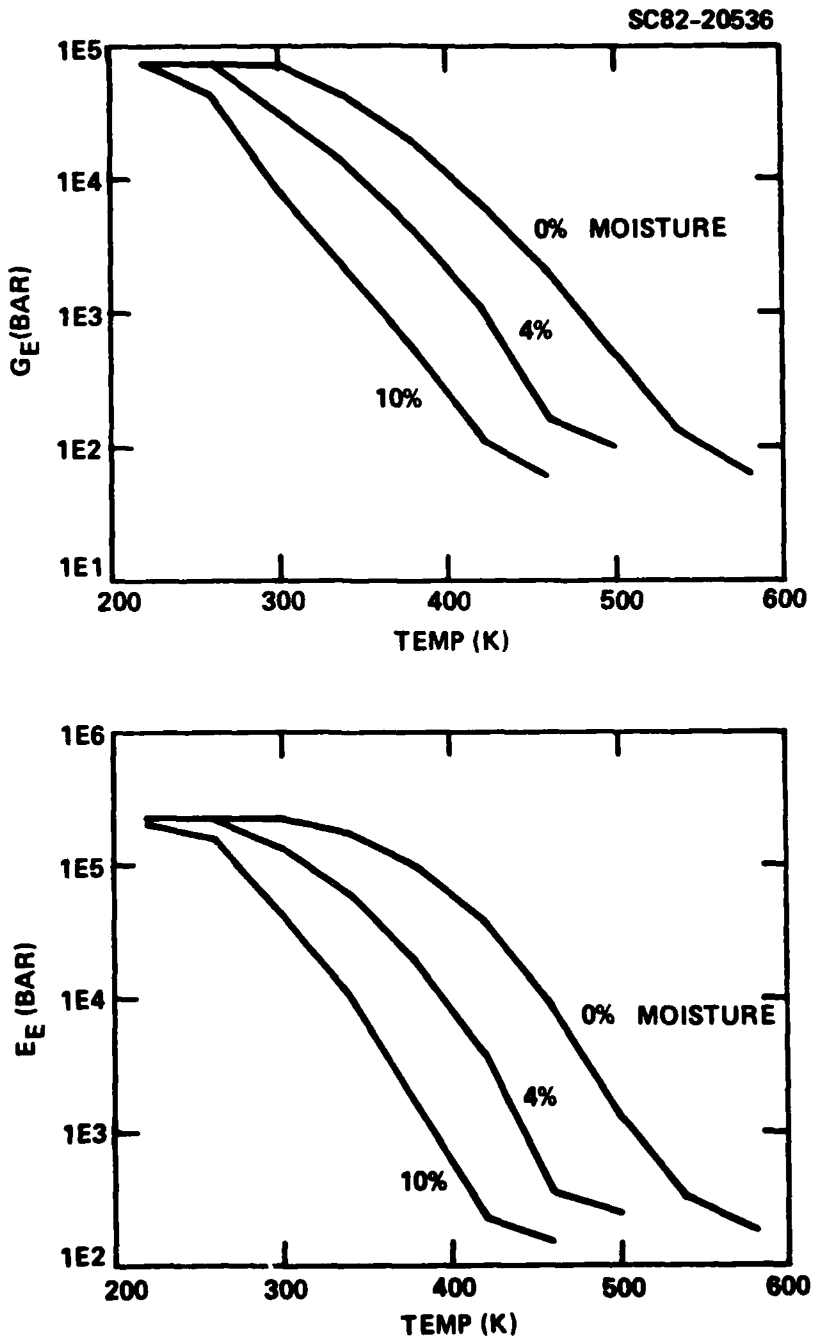


Fig. 6-13 Calculated engineering shear modulus (upper) and tensile modulus (lower curves) for cured epoxy with varied wt% moisture.

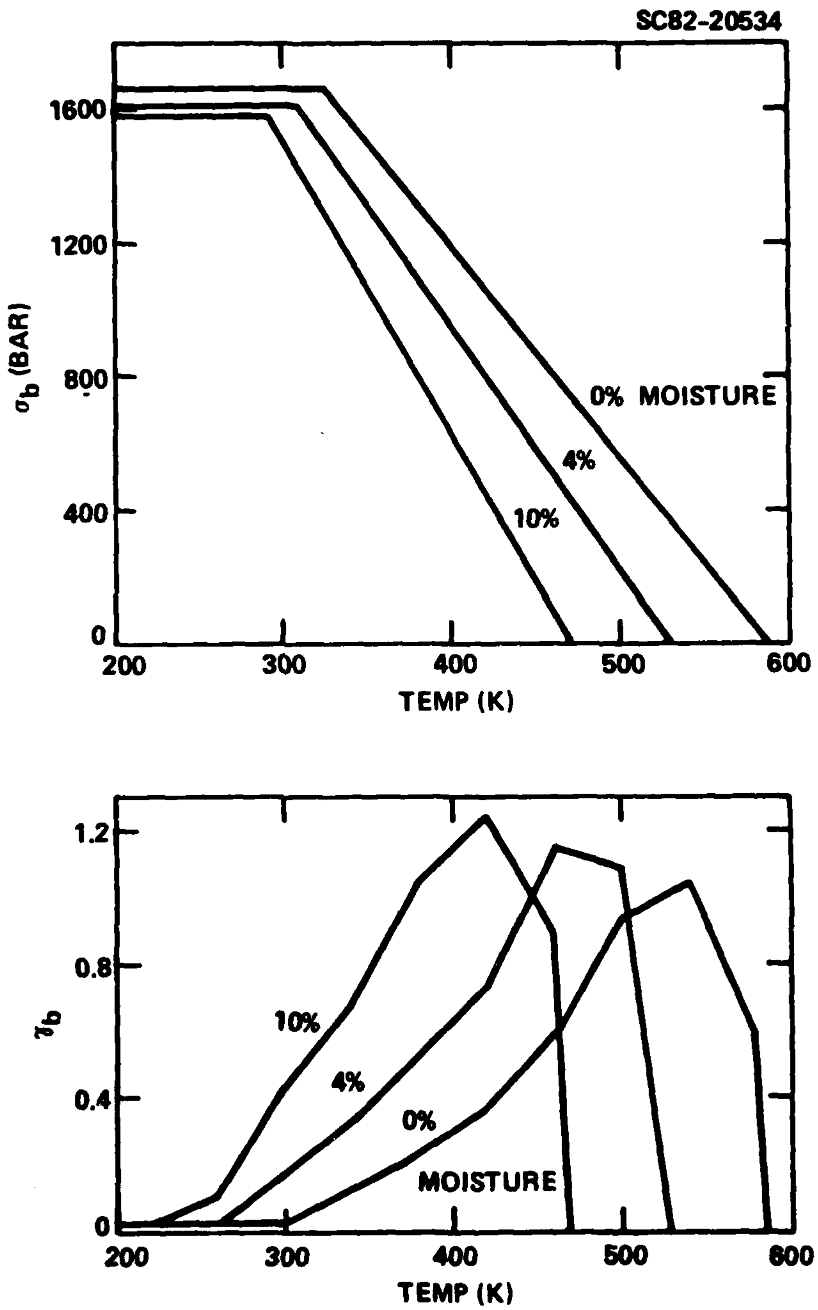


Fig. 6-14 Calculated shear strength (upper) and shear extensibility (lower curves) for cured epoxy with varied wt% moisture.

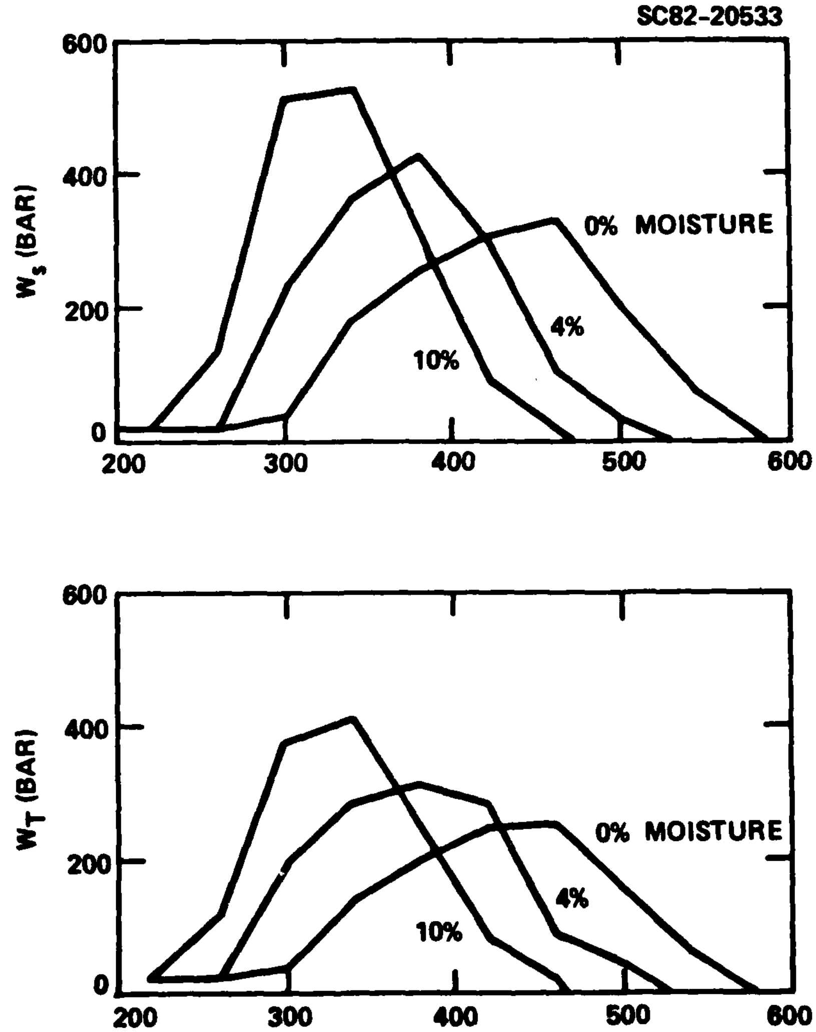


Fig. 6-15 Calculated specific fracture energy in shear (upper) and tension (lower curves) for cured epoxy with varied wt% moisture.

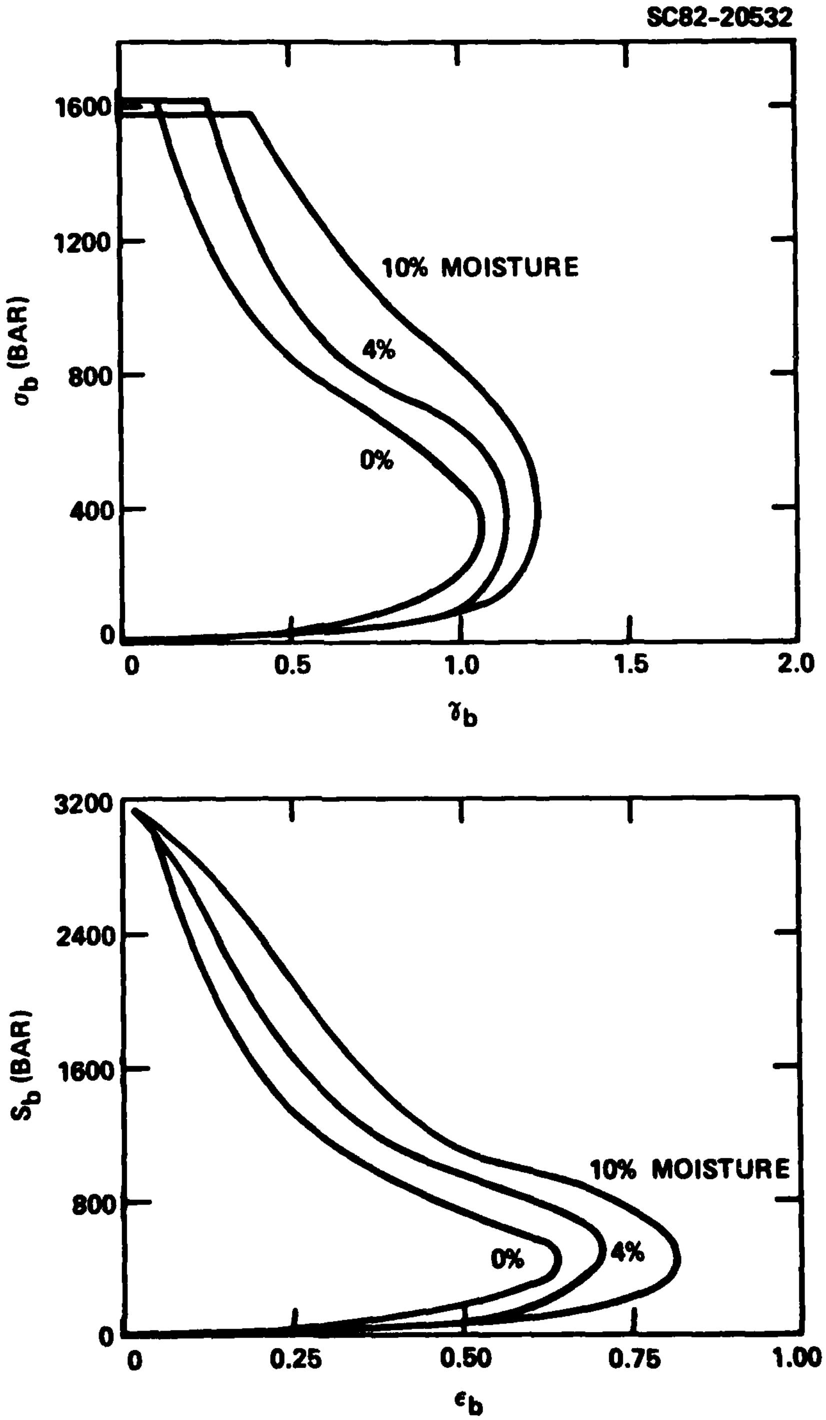


Fig. 6-16 Calculated failure envelopes in shear (upper) and tension (lower curves) for cured epoxy with varied wt% moisture.

SC83-20656

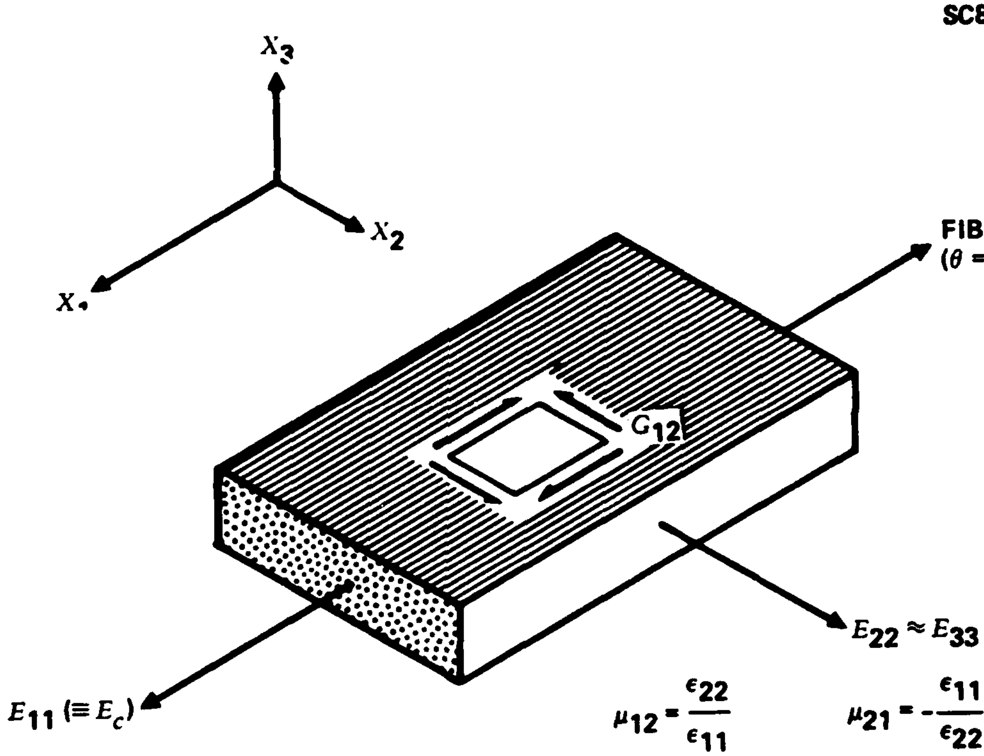


Fig. 6-17 Unidirectional reinforced composite.

SC83-20660

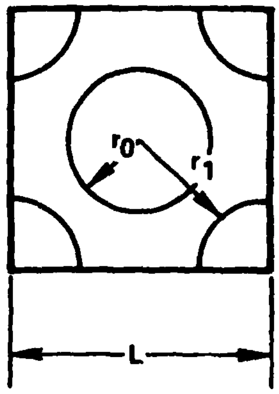
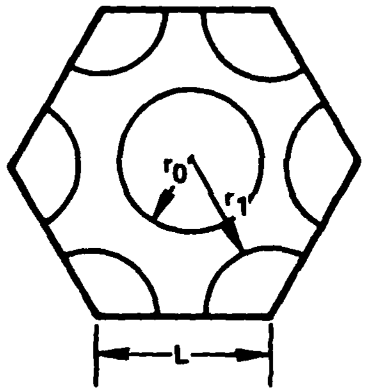
LATTICE TYPE	SQUARE	HEXAGONAL
UNIT GEOMETRY		
FIBERS/UNIT CELL	2.0	3.0
FIBER VOLUME FRACTION (v)	$2\pi(r_0/L)^2$	$1.1548\pi(r_0/L)^2$
UNIT CELL AREA (A)	$2\pi r_0^2/V$	$3\pi r_0^2/V$
$a = (r_1 - r_0)$	$r_0[(\pi/V)^{1/2}-2]$	$r_0[1.074(\pi/V)^{1/2}-2]$
v AT $(r_1 - r_0) = 0$	0.785	0.906

Fig. 6-18 Packing geometries for regular uniaxial fiber arrays.

SC83-20658

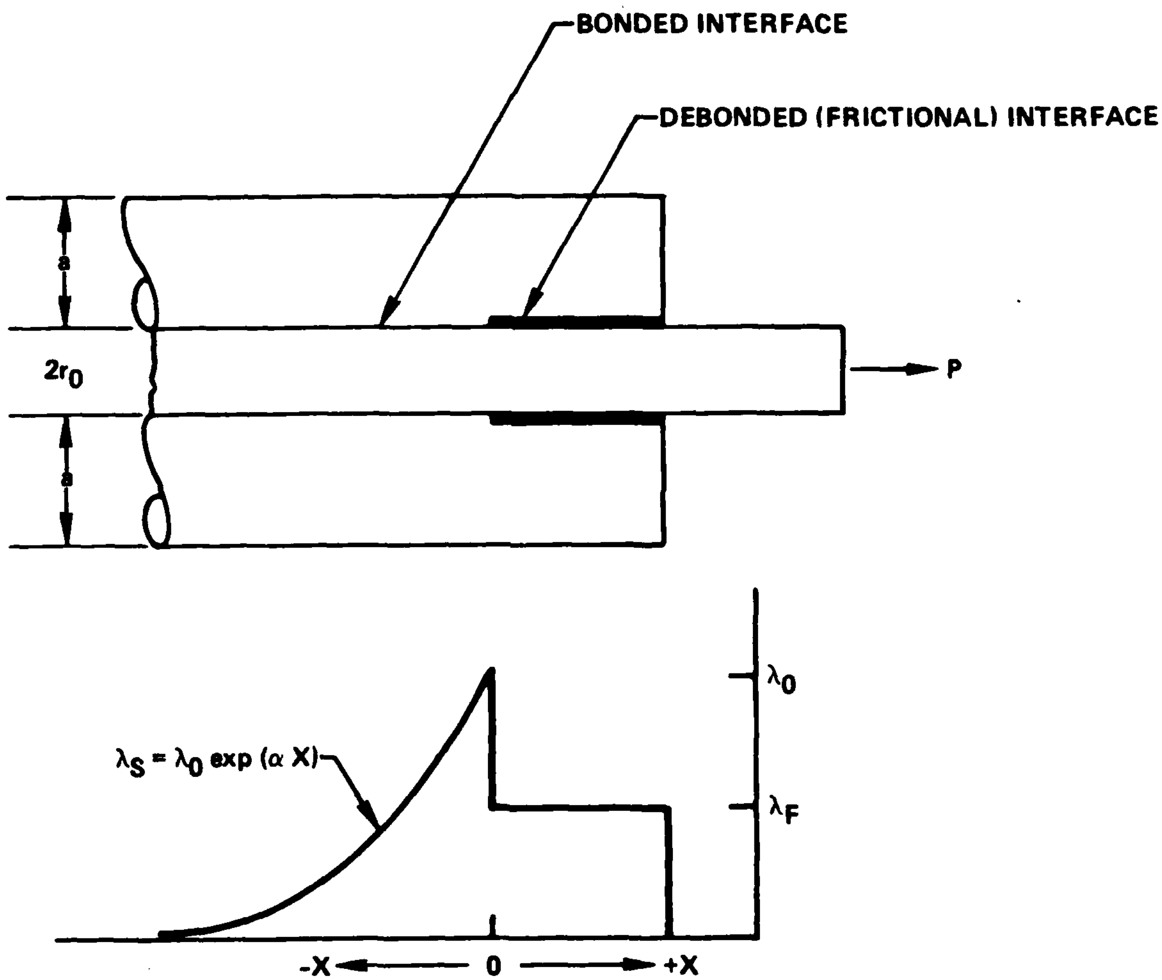


Fig. 6-19 Frictional (λ_F) and bonded (λ_S) interfacial shear stresses during fiber pull-out.

SC83-20655

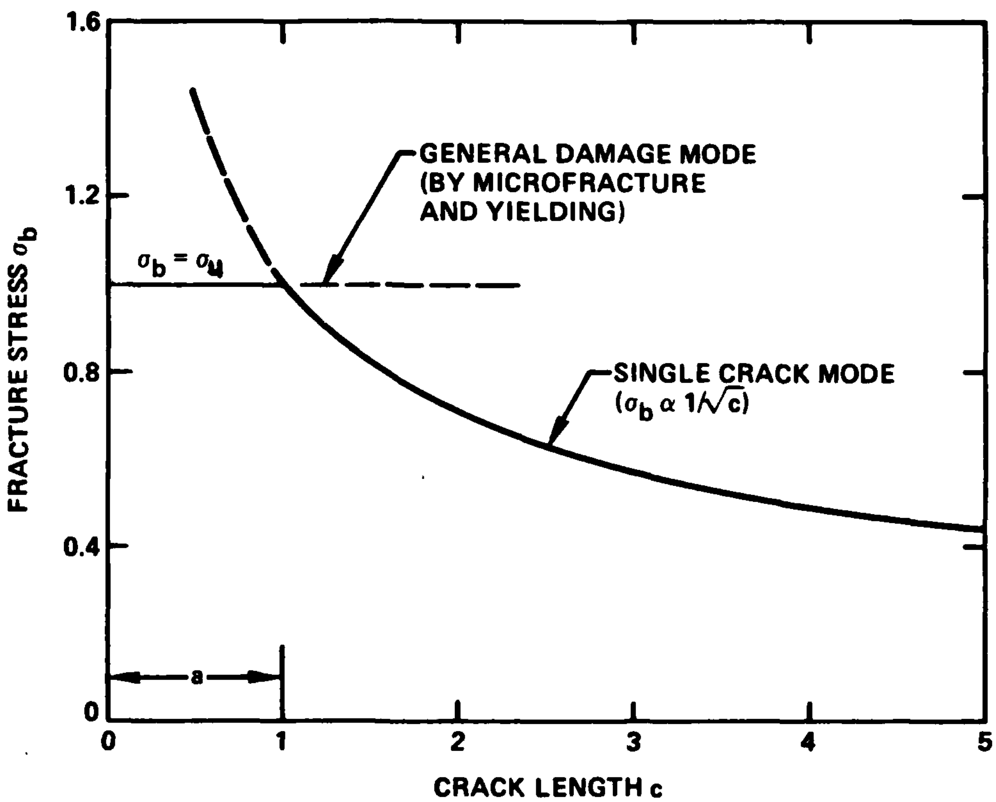


Fig. 6-20 Schematic showing the observed variation in failure mode and fracture stress σ_b with crack length c in damage tolerant composites.

SC83-20659

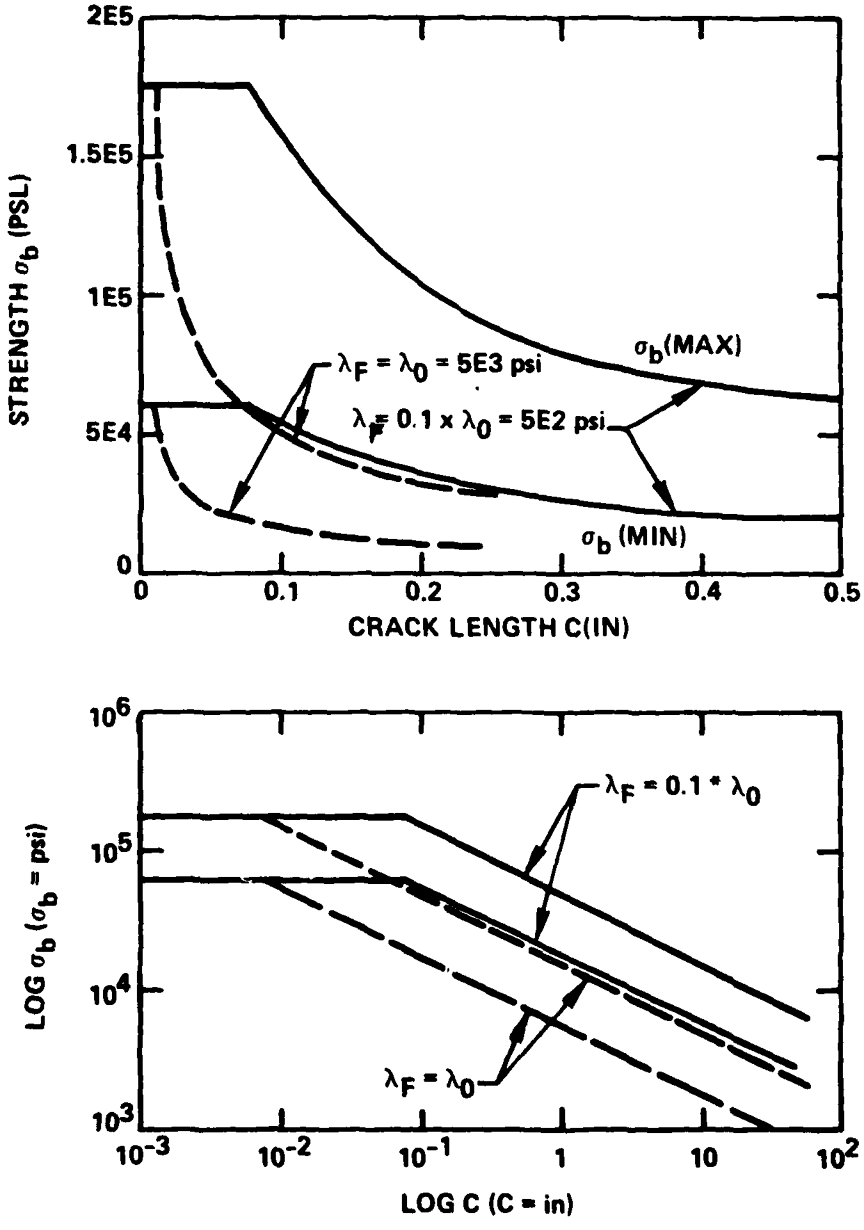


Fig. 6-21 Calculated curves of composite strength maximum σ_b(max) and minimum σ_b(min) vs crack length c.

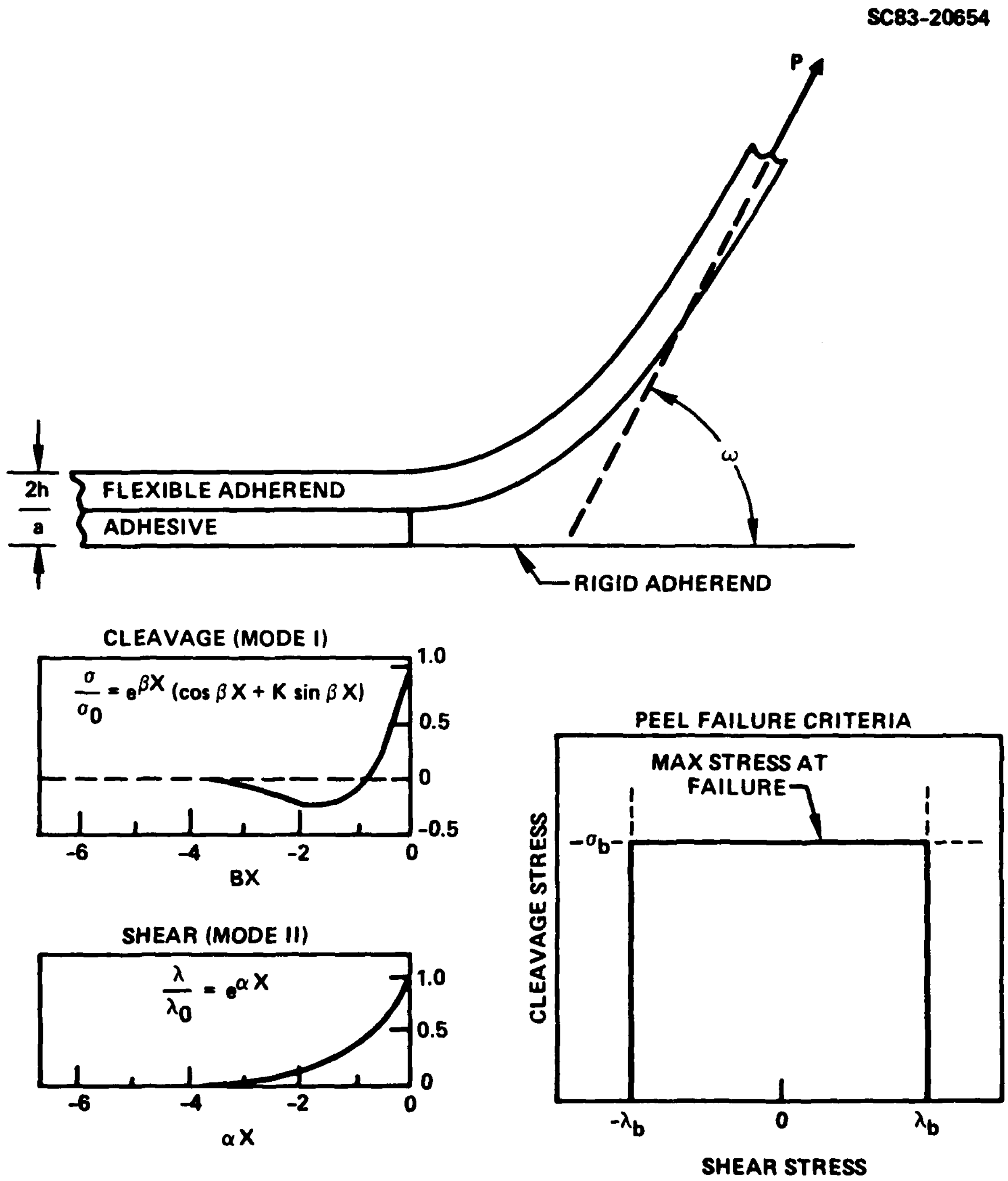


Fig. 6-22 Peel mechanics (upper and left views) and failure criteria.

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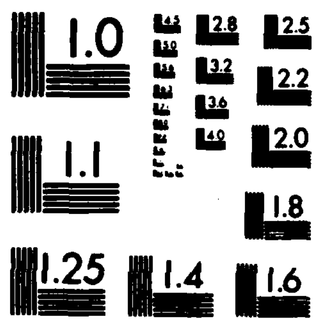

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NATIONAL BUREAU OF STANDARDS-1963-A

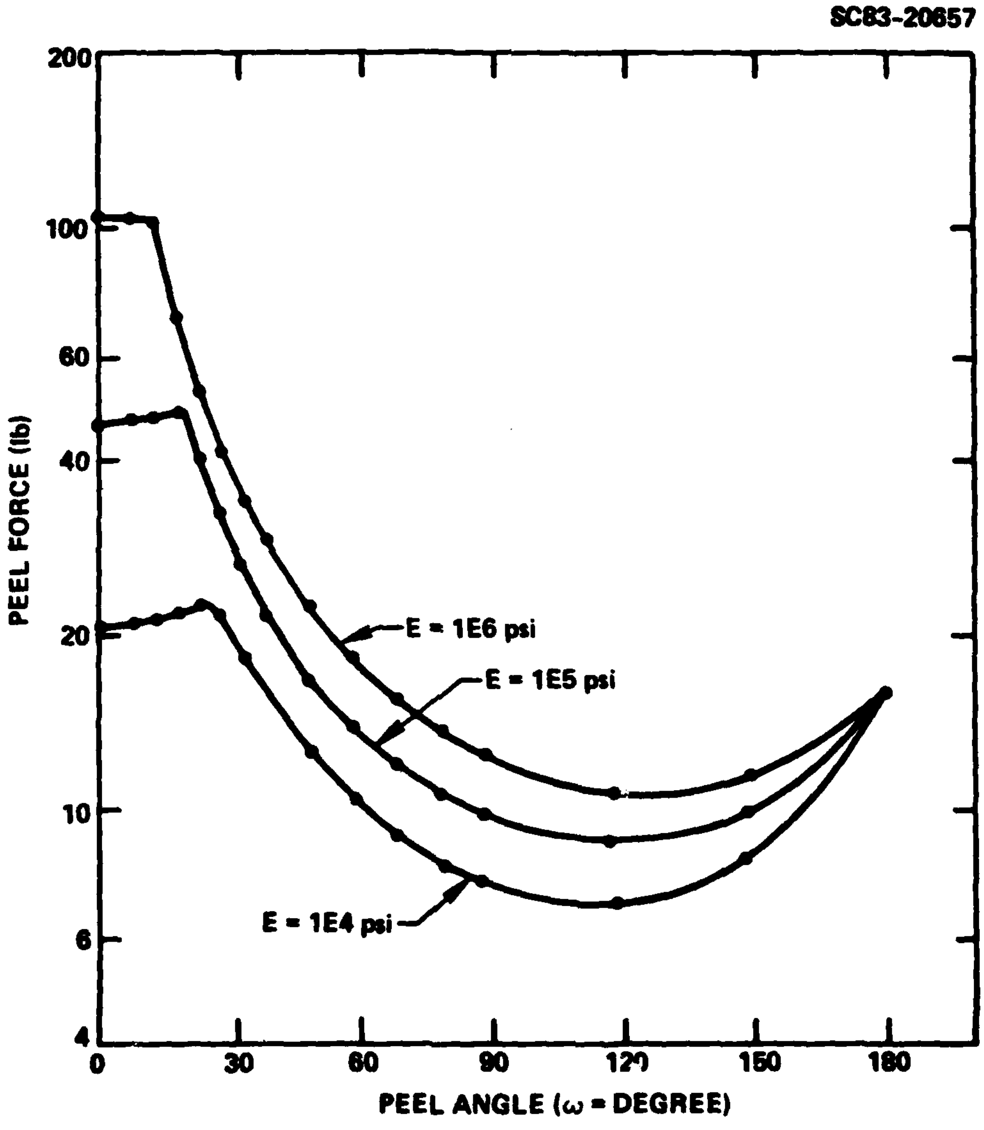

Fig. 6-23 Calculated curves of peel force P vs peel angle W for three values of flexible adherend tensile modulus E.